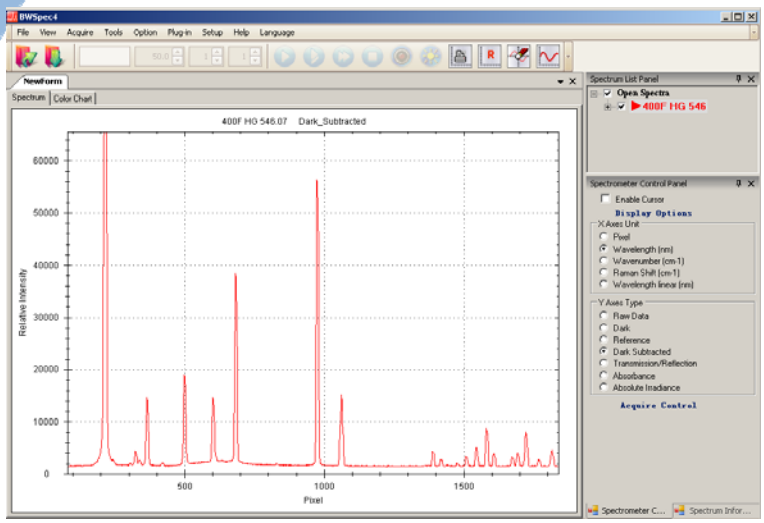
BWSpec 4



BWSpec 4

Array Spectrometer Acquisition Software

User Manual

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Tel: (302) 368-7824 · Fax: (302) 368-7830 · Email: www.bwtek.com/contact

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TABLE OF CONTENTS

1. Introduction 4
2. Installation 4
2.1. Operating Systems Supported 4
2.2. Installation 4
3. Software Main Screen 4
3.1. Menu bar 5
3.2. Tool bars 15
3.3. Spectrum List Panel 16
3.4. Spectrometer Control Panel 16
3.5. Spectrometer Info Panel 17
3.6. Status bar 18
4. Spectrum Display 18
4.1. Show In Overlay Mode 18
4.2. Show In Sequence Mode 18
4.3. Spectrum Display Setting 19
4.4. Spectrum Color Setting 20
4.5. Spectral Graph Setting 21
5. Spectrum View 22
5.1. Zoom In 22
5.2. Pan 22
5.3. Restore of View 22
5.4. Restore the Initial View 23
5.5. Copy and Save the Spectrum as an image 24
5.6. Show Values 24
6. Spectral Processing 25
6.1. Spectral Smoothing 25

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6.2. Peak Analysis 26
7. Save and Import Spectrum 28
7.1. Save A Single Spectrum 28
7.2. Save All Spectra Into ZIP file 28
7.3. Save All spectra To One File Folder 28
7.4. Import Spectrum 29
8. Read Flash 29
9. Plug-in 29
9.1. Background Removal 30
9.2. Export Data 31
9.3. Derivative 32
9.4. Timeline 33
9.5. Linearity Correction 36
9.6. Relative Intensity Correction 38
9.7. Reference Materials Correction 42
9.8. Absolute Irradiance 44
9.9. Color Measurement 49
Appendix A: Irradiance Ratio File Data Definition 59
Appendix B: Definition of Irradiance Data File Format 61

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1. Introduction

BWSpec is a spectrometer data acquisition operating software program used for B&W Tek spectrometers.

2. Installation

2.1. Operating Systems Supported

- 32 bit Windows Operating Systems, including:
  Windows 98/98 Second Edition
  Windows ME
  Windows NT 4
  Windows 2000/XP
  Windows Vista
  Windows 7
- 64 bit Windows Operating Systems, including:
  Windows XP
  Windows 7

Select an applicable installation package before proceeding with the installations.

2.2. Installation

Insert the BWSpec4 CD into the disc tray. An installation screen will appear for installation procedures. Follow the installation instructions through the install wizard. After BWSpec4.00 is installed successfully, a shortcut icon will be created automatically on the desktop.

3. Software Main Screen

Spectrometer Models with USB Interfaces

- Connect the spectrometer to USB Port of computer via USB Cable.
- Launch BWSpec.exe by clicking the shortcut icon on the Desktop. From the BWSpec4.00 Menu bar: **Tools → Flash Access,**
- Click **Read Flash**, and the unit specific parameters for the unit will be read from the spectrometer to the BWSpec settings through the USB connection.

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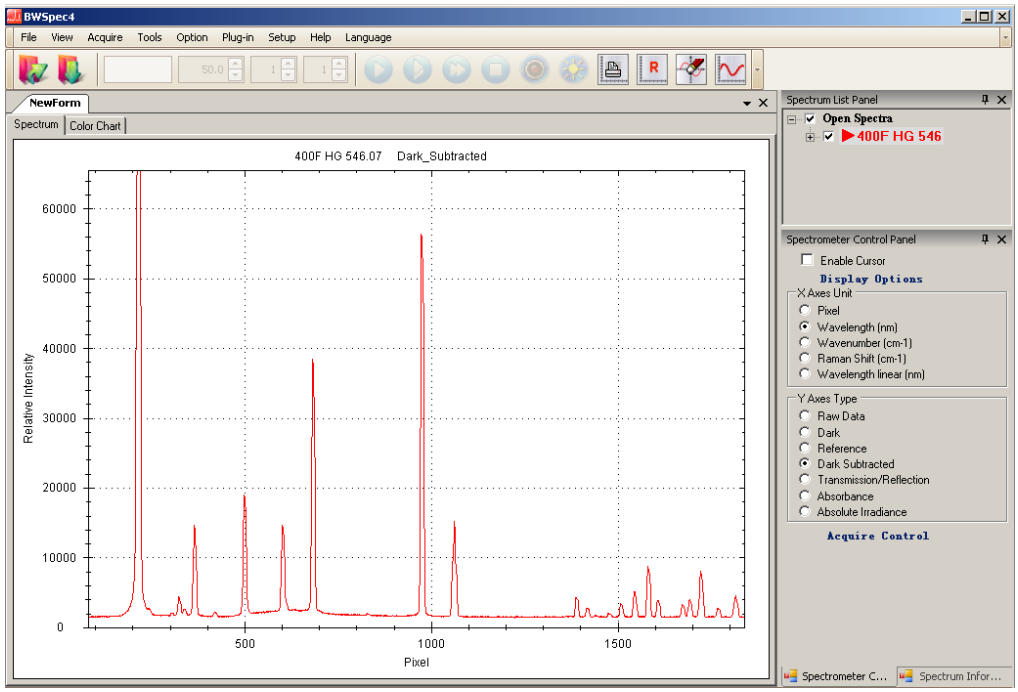
- After the “Read Flash Completed” message appears, click “Close” button on the bottom right.
- The spectrometer is now successfully set up to the connected computer for operation.



BWSpec 4 Main User Interface Screen

3.1. Menu bar

3.1.1. File

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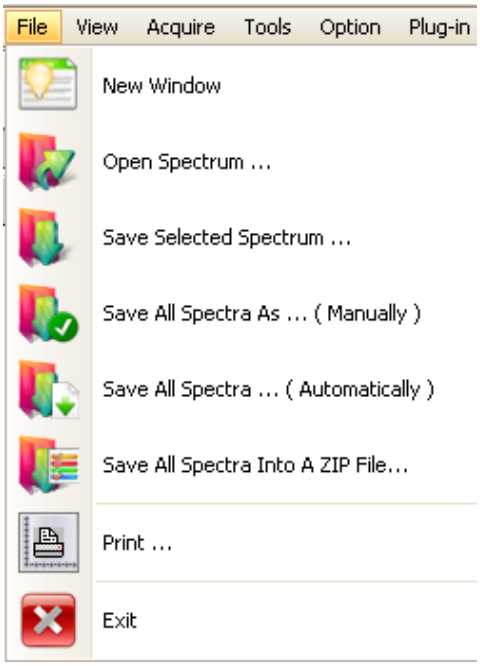

- Create New Window
  Click **New Window** to create a new window of graph display with applicable panel for use with all available functions. This is a useful tool when loading a saved spectrum for reference or comparison purpose against acquired spectra in separate graphs.

- Open Spectrum
  Click **Open Spectrum** to load one or more spectral files into the graph display.

  Data Format:
  BWSpec Data File (*.BwRam)
  TXT File (*.txt)
  SPC File (*.spc)
  BWSpec Data ZIP File (*.BwRamS)

- Save Selected Spectrum
  This is for saving the selected spectrum to a folder as specified.

  Data Format:
  TXT file (*.txt)

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CSV file (*.csv)
TXT file (even)
SPC file (*.spc)
BWTek Raman data file format (*.BwRam)

- Save All Spectra Into A Zip File
  Use this option to save all spectra to a zip file.

  Data Format:
  BWSpec Data ZIP File (*.BwRamS)

- Save all Spectra Automatically
  Menu option for saving all spectra into a specified file folder at one time, with each spectrum being saved as a single file inside this folder.

- Save all Spectra Manually
  Menu option for saving all spectra into a specified file folder, each spectrum is created as a single file inside this folder. The files are named in sequence as SP_0.txt, SP_1.txt, …, SP_4.txt, etc. But you can also change the file names manually.

- Print Preview
  To view the current spectrum on screen as it would appear on the print out.

- Exit
  To exit BWSpec 4. A message will be shown if there is a spectrum that has not been saved before exiting the software.

3.1.2. View

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- Show In Overlay
  To display spectra in one graph as overlays.

- Show In Sequence
  To display one spectrum in a graph with a sequence of graphs.

- Spectrum List Panel
  This option is for activating a list panel. This panel after being enabled lists sequentially all captured spectra. A spectrum becomes active after it is selected from the list. Otherwise an active spectrum is the last one acquired.

- Spectrum Info Panel
  This option is for activating a spectrometer info panel. This panel displays associated operation setting parameters such as integration time used and average time used to the active spectrum.

- Spectrometer Control Panel
  This menu option is for a control panel to be displayed for configuring the graph display options. Refer to 3.4 for details.

3.1.3. Acquire

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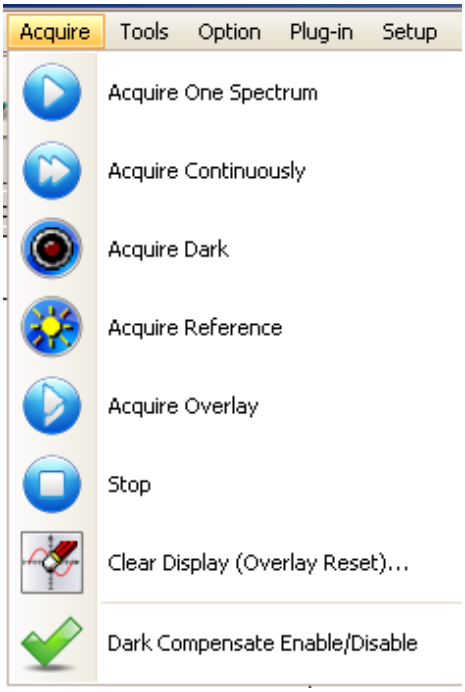
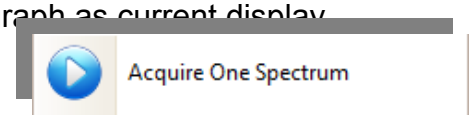
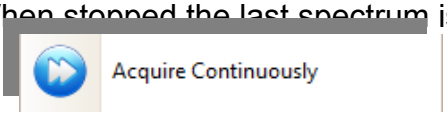


- Click **Acquire One Spectrum** to acquire a new spectrum and update to the graph as current display.

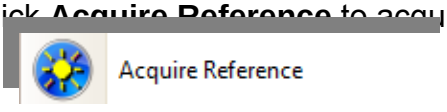


- Click **Acquire Continuously** to acquire new spectra in a live mode continuously. When stopped the last spectrum is updated to the current graph.



- Click **Acquire Dark** to acquire a new spectrum for use as a dark scan.

- Click **Acquire Reference** to acquire a new spectrum for use as a reference scan.



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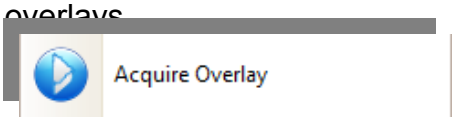
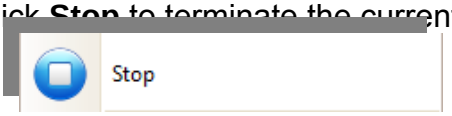
- Click **Acquire Overlay** to capture a new spectrum and add to the current graph in overlays.



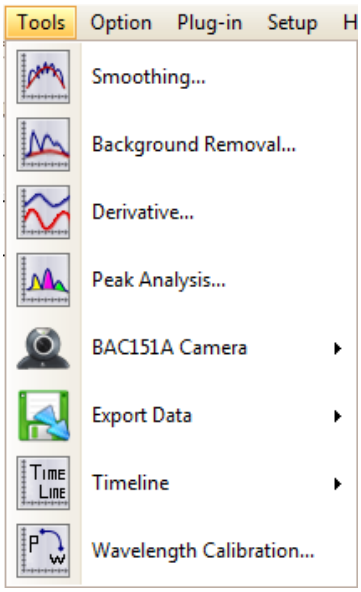
- Click **Stop** to terminate the current acquisition in progress.



- Click **Clear Display** to clear all spectra displayed from the current graph display.

- Click **Dark Compensate Enable/Disable** to turn on or off the electronic dark reference that are available with some detector arrays for automatic dark subtractions based on those available references.

3.1.4. Tools



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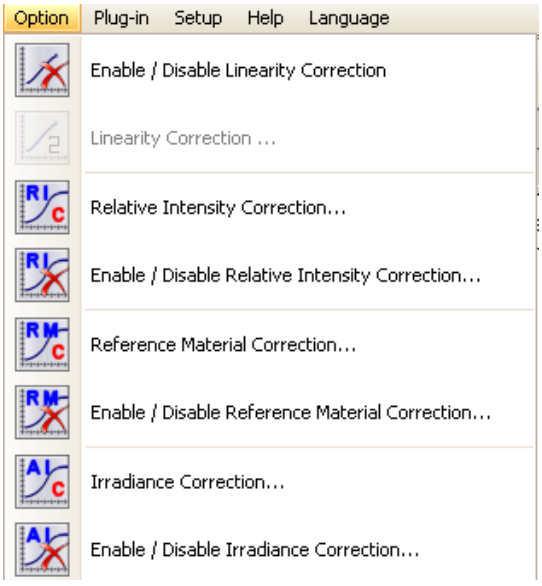
- Click **Smoothing** to open the Smoothing option dialog box. Refer to section 6.1 for more details
- Click **Background Remove** to remove the fluorescence background using an automated algorithm for Raman spectral analysis
- Click **Derivative** to apply derivative operation to an active spectrum
- Click **Peak Analysis** to open the Peak Analysis dialog box. Refer to 6.2 for more details.
- Click **BAC151A Camera** to enable the video camera support for BAC151A accessory (for Raman analysis option only)
- Click **Export Data** to export collected spectrum into txt file.
- Click **Timeline** for programmed spectral data recording.
- Click **Wavelength Calibration** to enter wavelength calibration functions.

3.1.5. Option



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- Click **Enable / Disable Linearity Correction** to enable or disable linearity correction function. A unit specific correction file will need to be supplied in order for the correction to work correctly.

- Click **Enable / Disable Relative Intensity Correction** to enable or disable relative intensity correction function. This is a function related to correcting the unit spectral response against a known reference. A unit specific correction file will need to be supplied in order for the correction to function.

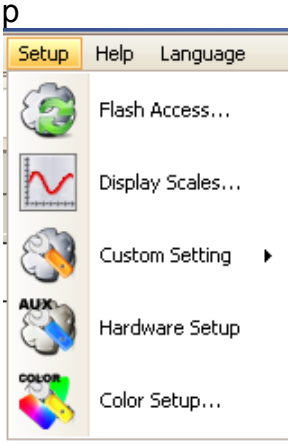
- Click **Enable / Disable Reference Material Correction** to enable or disable reference material correction function. This function is useful for accurate measurements in applications such as percent reflectance. A reference material with certified reference value file will be needed in order for the correction to work accurately.

- Click **Enable / Disable Irradiance Correction** to enable or disable irradiance correction function. A unit specific correction file will need to be supplied in order for the correction to work correctly.

3.1.6. Plug-in

Click **Plug-in** to open the **Plug-in Manager** dialog box, where all available plug-ins are listed. Check corresponding box to choose the plug-in functions you need. Click **Apply** and then **OK**. The settings with checked plug-ins will be saved automatically.

3.1.7. Setup



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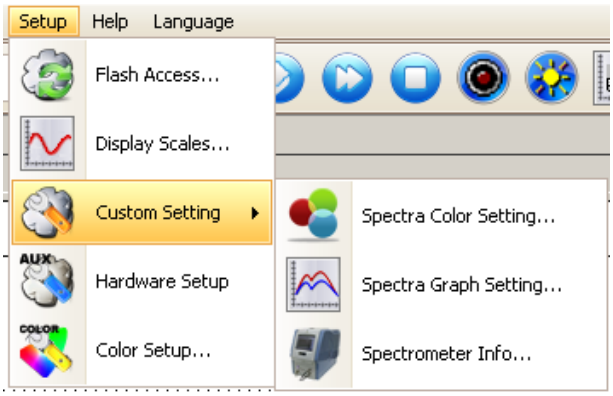
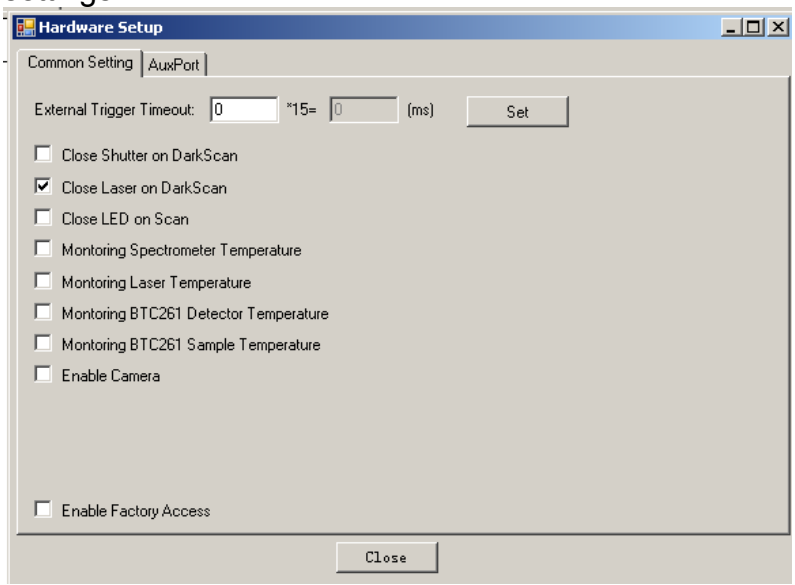
- Click **Flash Access** to access the spectrometer specific info associated with the currently connected spectrometer.

- Click **Display Scales** to configure the X/Y settings and scales.

- Click **Custom Setting** for custom spectral settings including Spectra Color Setting, Spectral Graph Setting, as well as access to the spectrometer info for the currently connected spectrometer.



- Click **Hardware Setup** for spectrometer common settings as well as AuxPort settings.



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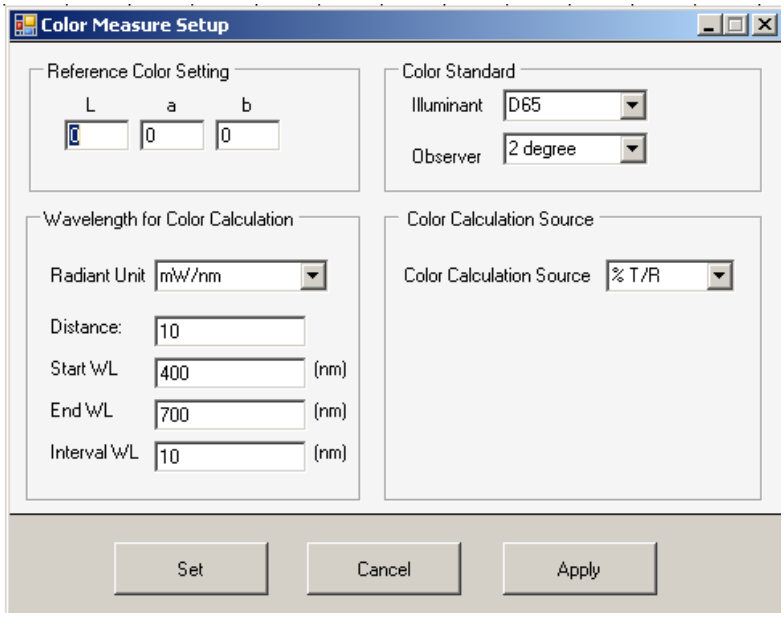
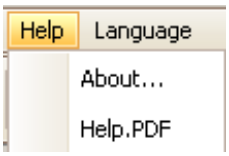
- Click Color Setup for color measurement function settings.



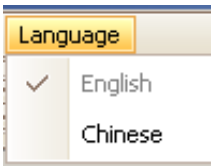
3.1.8. Help

- Click **Help** → **About** to find out the current version of the software
- Click **Help** → **Help.PDF** to display the User Manual of the BWSpec 4 software



3.1.9. Language

Click **Language** to select a display language desired for the software: **English** or **Chinese.**



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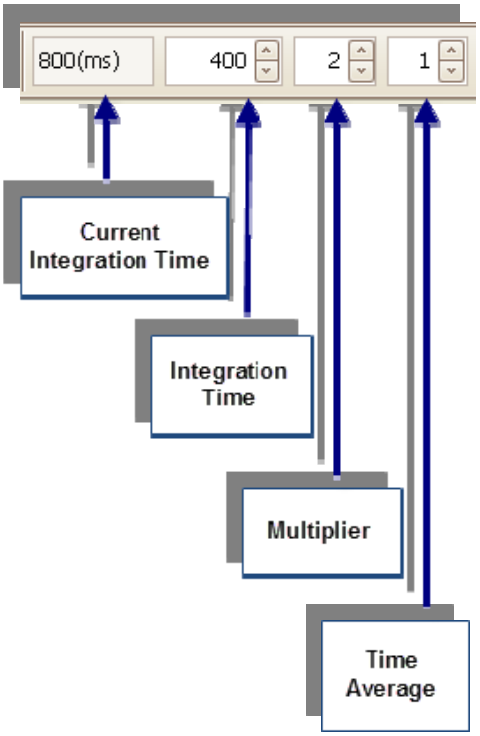
3.2. Tool bars

Open spectrum

Save spectrum



This bar is for operation parameter setting, including current integration time, integration time, multiplier, and time average.

Current Integration Time
= Integration Time * Multiplier

These buttons are for spectrum acquisition. Refer to 3.1.3 for details.

Print spectrum

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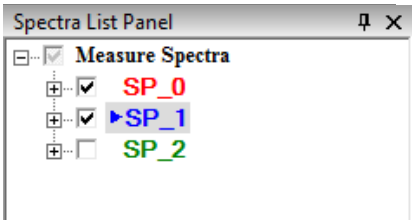
Reset the scale

Delete all current imported and acquired spectra.

Set the X & Y-axis unit and scale.

3.3. Spectrum List Panel

Spectrum List Panel is located on the top-right side of the main screen after being activated.



The spectra with √ signs indicate that the spectra are selected for being displayed in the current graph, while the spectra without the signs are hidden from the current graph display. The spectrum with ▶ indicates the currently active spectrum selected.

3.4. Spectrometer Control Panel

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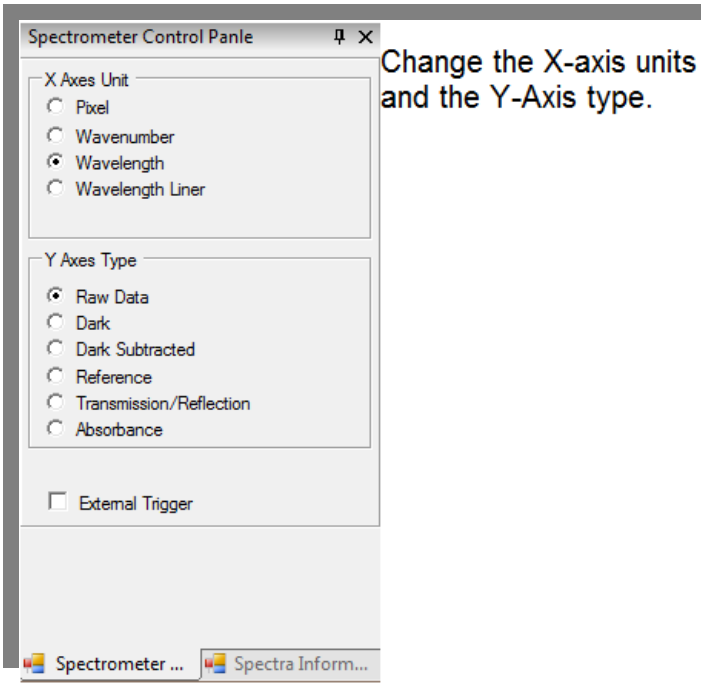
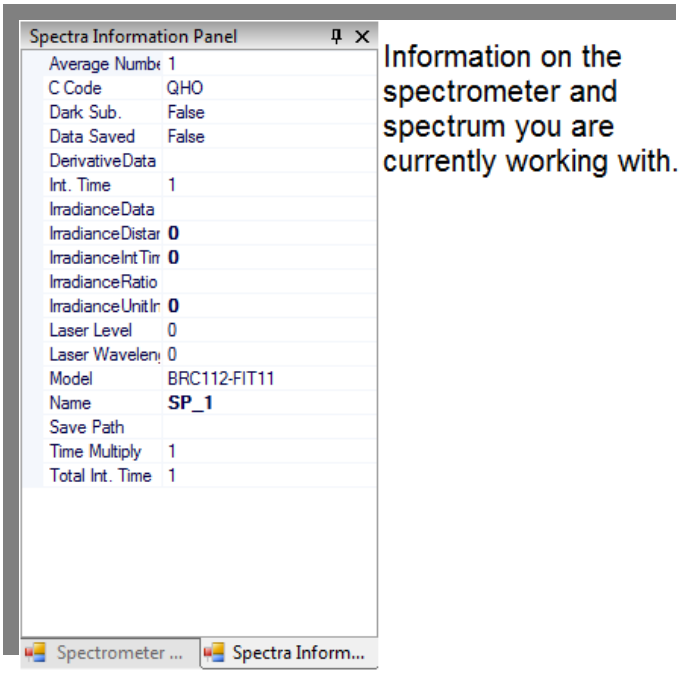


Change the X-axis units and the Y-Axis type.

3.5. Spectrometer Info Panel



Information on the spectrometer and spectrum you are currently working with.

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3.6. Status bar

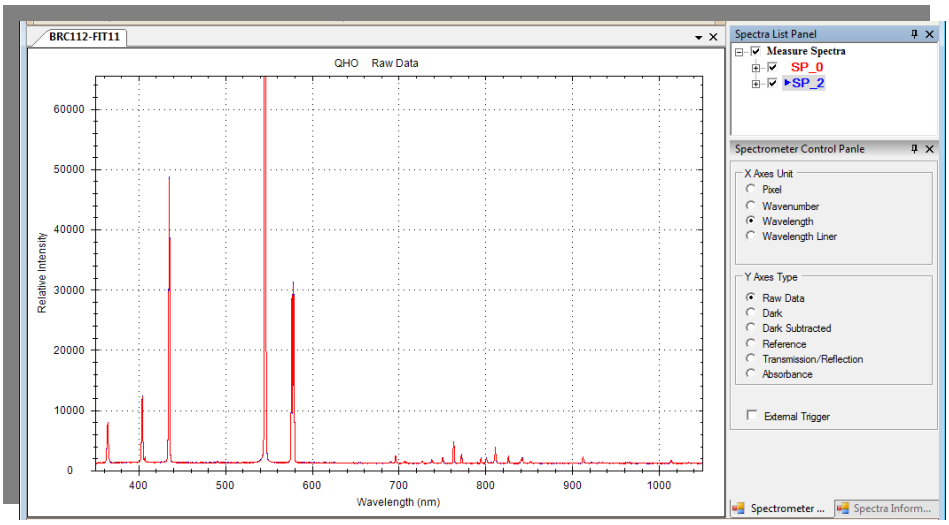
4. Spectrum Display

A spectrum can be displayed in two modes:

- Show In Overlay
- Show In Sequence

4.1. Show In Overlay Mode

Click **View** on the menu bar and select **Show In Overlay**.



4.2. Show In Sequence Mode

Click **View** on the menu bar and select **Show In Sequence**.

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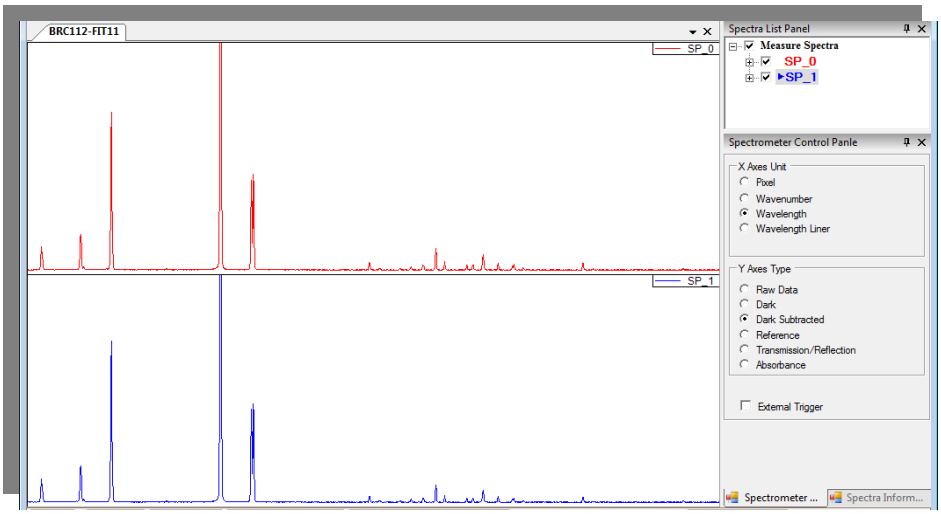
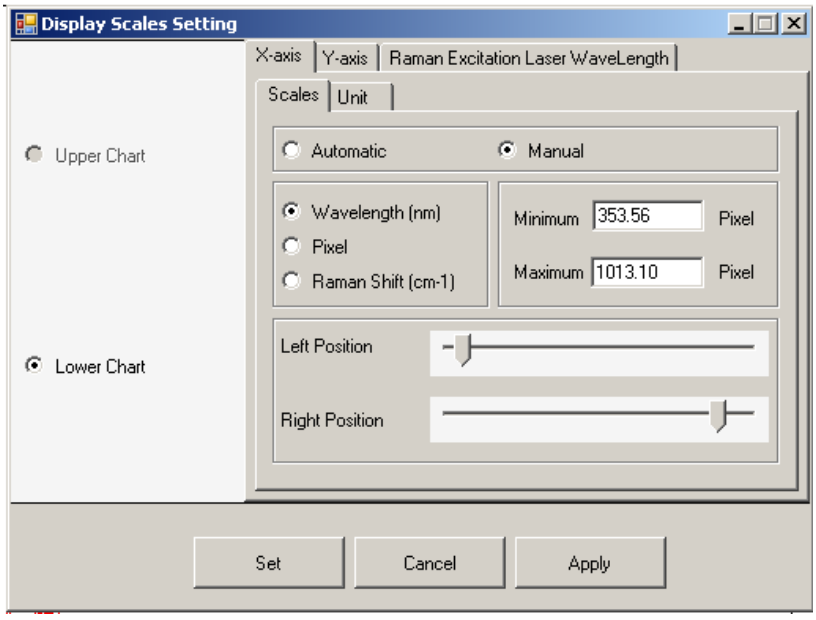


4.3. Spectrum Display Setting

On the menu bar click **Setup** → **Display Scales**, or simply click on the tool bar. A dialog box will display, where the scale settings on both X and Y axis can be adjusted.



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4.3.1. Unit for X-axis

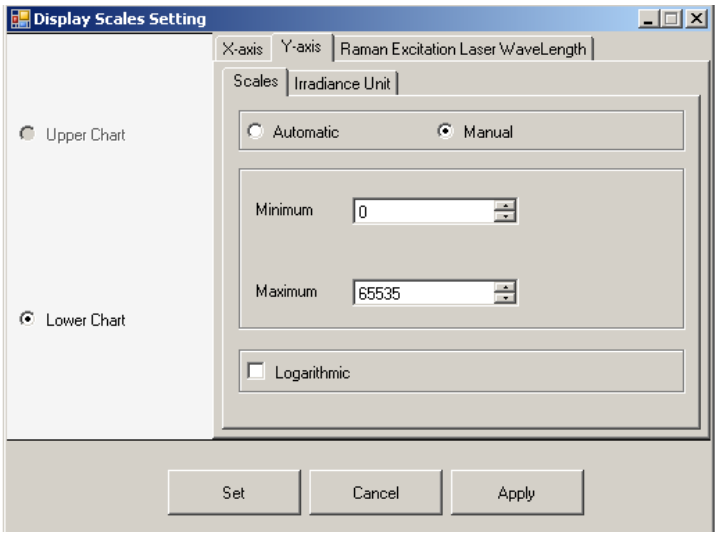
Click on X-axis tab, you can set X-axis to one of these three units:

- Wavelength (nm)
- Pixel
- Raman Shift (cm^{-1})

4.3.2. Unit for Y-axis

Click on Y-axis tab, you can set the Y-Axis to:

- Automatic scale
- Manual scale
- Logarithmic
- Irradiance unit (available when the function is enabled)



4.4. Spectrum Color Setting

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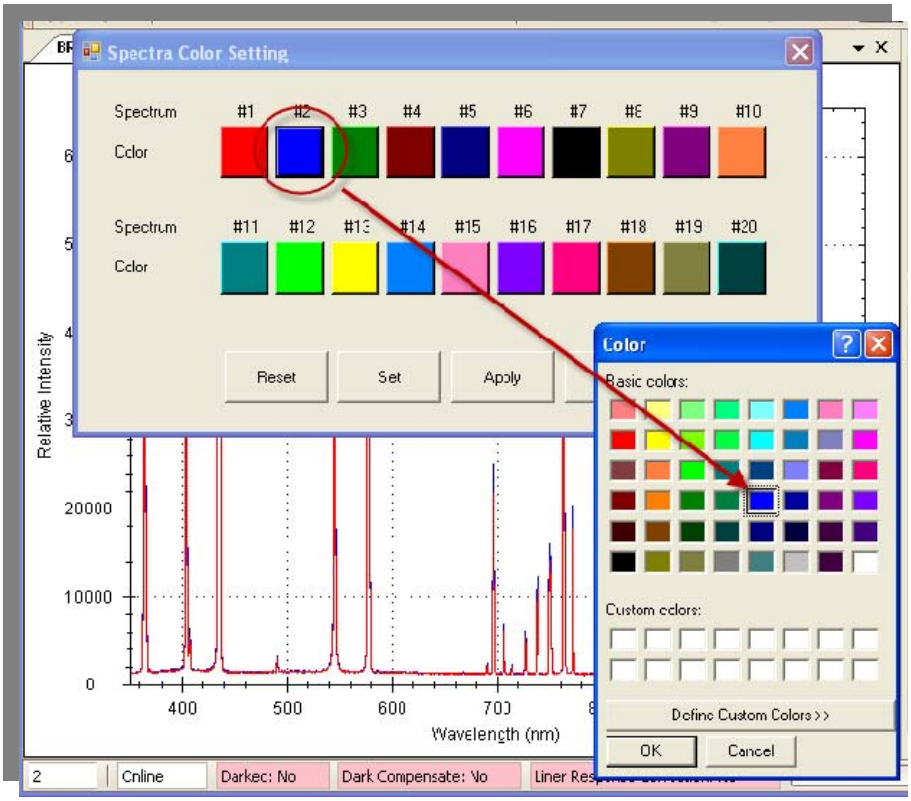
When more than one spectrum is displayed, each one will have a different color. Initially default colors will be assigned automatically to each spectrum on the spectrum display panel. The colors can be manually changed to designed ones by following the below procedure.

On the menu bar, click **Setup** → **Custom Setting** → **Spectra Color Setting**



Click on the # of the spectrum you'd like to change, choose color, click **OK**, and **Apply**. Click **Set** to save the setting, or **Close** to close the window without saving the setting.

4.5. Spectral Graph Setting

Spectral Graph Setting is for configuring the graph background color, spectrum display line width, and font size in the graph area.

On the menu bar, click **Setup** → **Custom Setting** → **Spectra Graph Setting**

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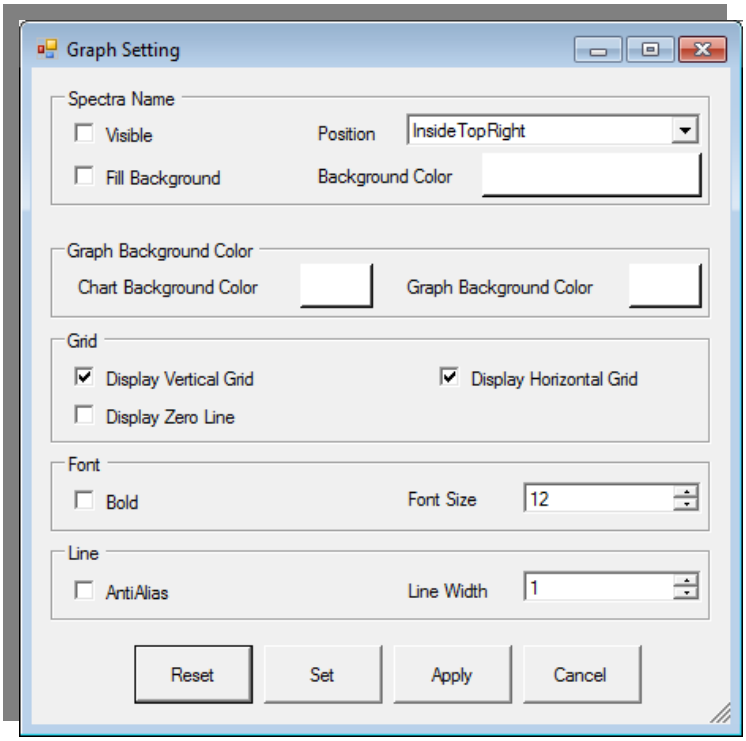
A dialog box will show where spectral graph settings can be adjusted.



5. Spectrum View

5.1. Zoom In

To zoom in a spectrum, hold down the left mouse button and drag the cursor to make a box around the area you wish to zoom in on.

5.2. Pan

Hold “Ctrl” key and hold down left mouse button, move the cursor in the direction of the area you wish to view.

5.3. Restore of View

Place cursor in the graph area, right click your mouse and select “Un-Zoom”, to zoom out.

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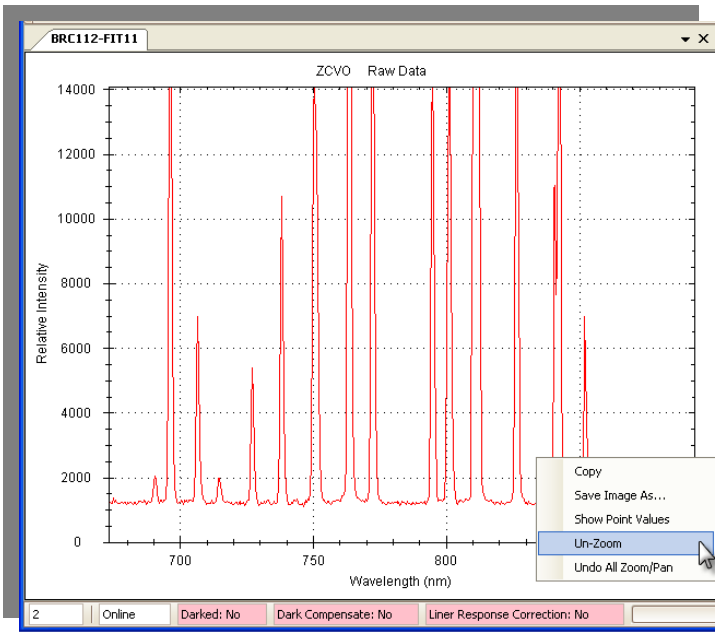
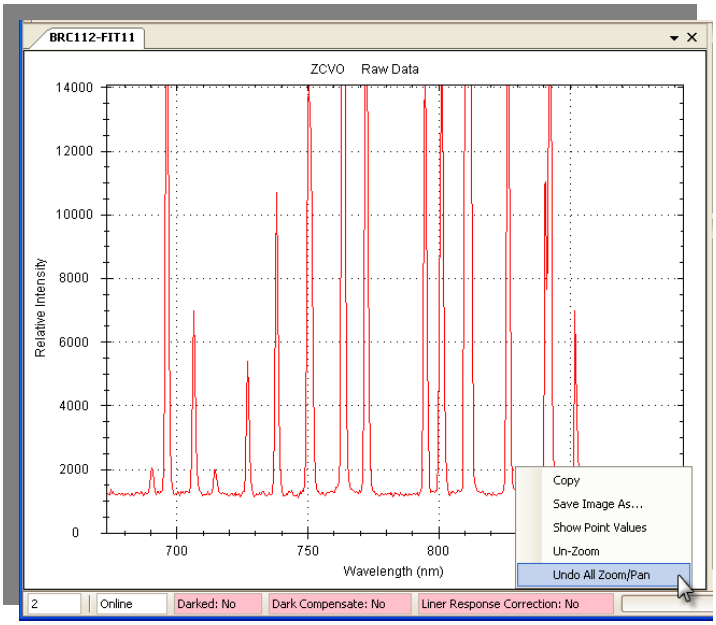


5.4. Restore the Initial View

Place cursor in the graph area and right click your mouse and select “Undo All Zoom/Pan”, to go back to original spectrum view.
You may also use the double-click of the left mouse for the same purpose.



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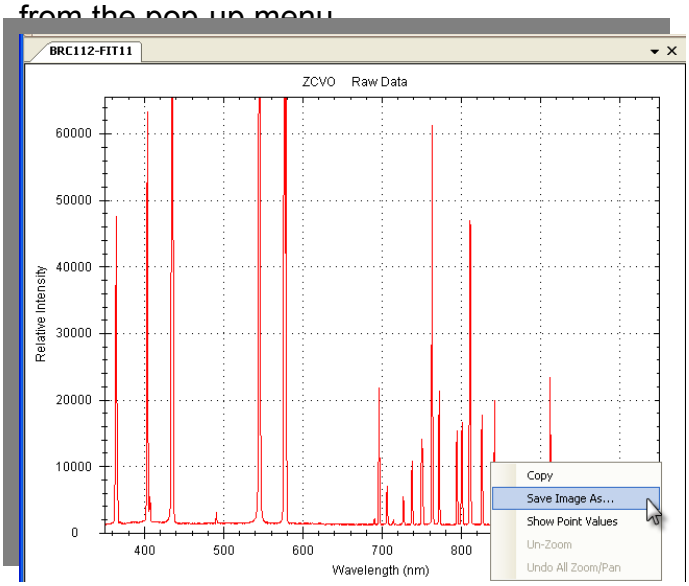
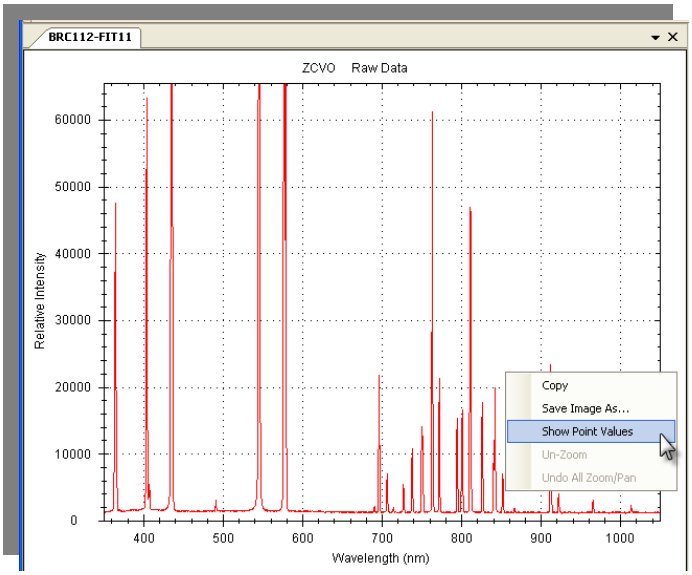
5.5. Copy and Save the Spectrum as an image

Place cursor in the graph area, right click to select “Copy” or “Save Image As” from the pop-up menu.



5.6. Show Values

Place cursor in the spectrum display area, right click to select “Show Values” from the popup menu. Values associated with the current data point of the spectrum in pixel, wavenumber, and wavelength will be displayed.



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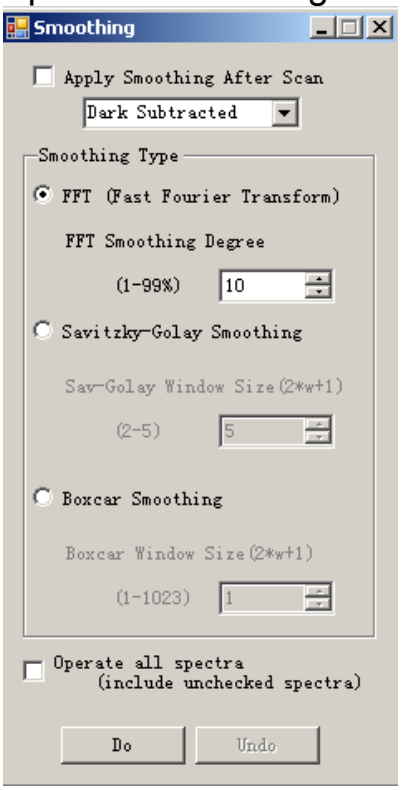
6. Spectral Processing

6.1. Spectral Smoothing



The Spectral Smoothing dialog box can be activated from menu bar **Tools**.
Three smoothing methods are provided in BWSpec4 for effective S/N enhancement:

- FFT (Fast Fourier Transform): smoothing can be applied to the original spectrum using a smoothing factor of in 1-99%. The smoothing factor needs to be carefully selected so that not to cause distorted spectrum.

- **Savitzky-Golay (Savitzky-Golay Filters):** smoothing can be applied to the original spectrum with a “window size” setting between 2-5. This is a very commonly used smoothing method with less chance to cause distortion and degradation to the spectral resolution.

- **Boxcar:** smoothing can be applied to the original spectrum using a “window size” setting in 1-1023. The smoothing function will apply the forward moving

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smoothing by taking the averaging of the specified number of pixels plus one pixel on the left to the group and one pixel to the right of the group. This is an effective smoothing operation at the expense of degraded spectral resolution, hence do not use a larger than necessary "window size" setting in order to preserve the needed spectral info.

FWHM is a useful tool for analyzing spectral features. When applied to the acquired narrow emission peaks such as peaks from low pressure mercury and argon lamps, the FWHM value can provide practical measure of the particular spectrometer spectral resolution.

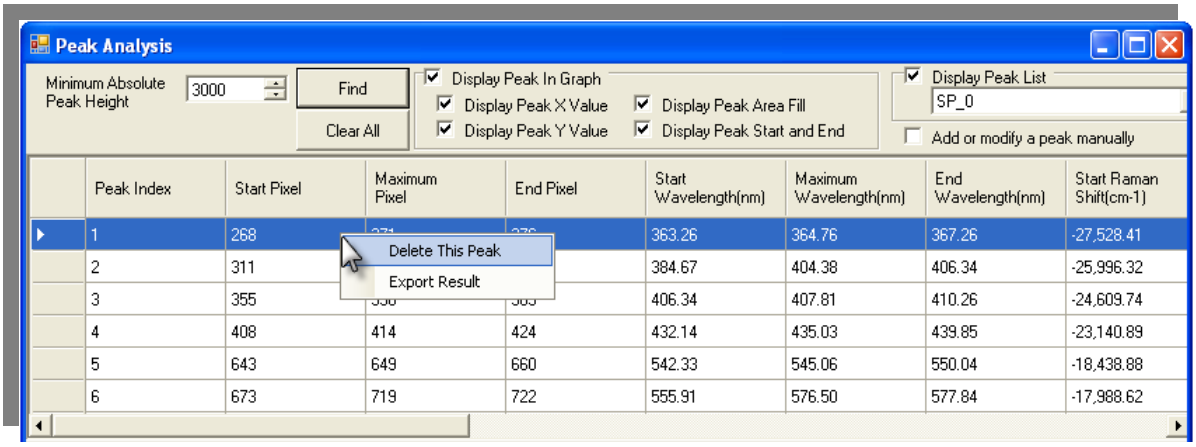
6.2. Peak Analysis

6.2.1. Automatic Peak Identification

From the menu bar, click **Tools → Peak Analysis**. The **Peak Analysis** window will appear. In the top left hand corner of the menu, input the value at **Minimum Absolute Peak Height** (threshold) and click **Find** to identify all peaks that exceed the threshold. All identified peaks are listed in a table in the window. This table provides you detailed information on the identified peaks. Check the box in front of **Display Peak In Graph** and the identified peaks will be marked on the spectrum.

6.2.2. Delete an Identified Peak

Right-click **Peak Index** for the peak you want to remove from the list and select **Delete This Peak**, and the removal will be done.



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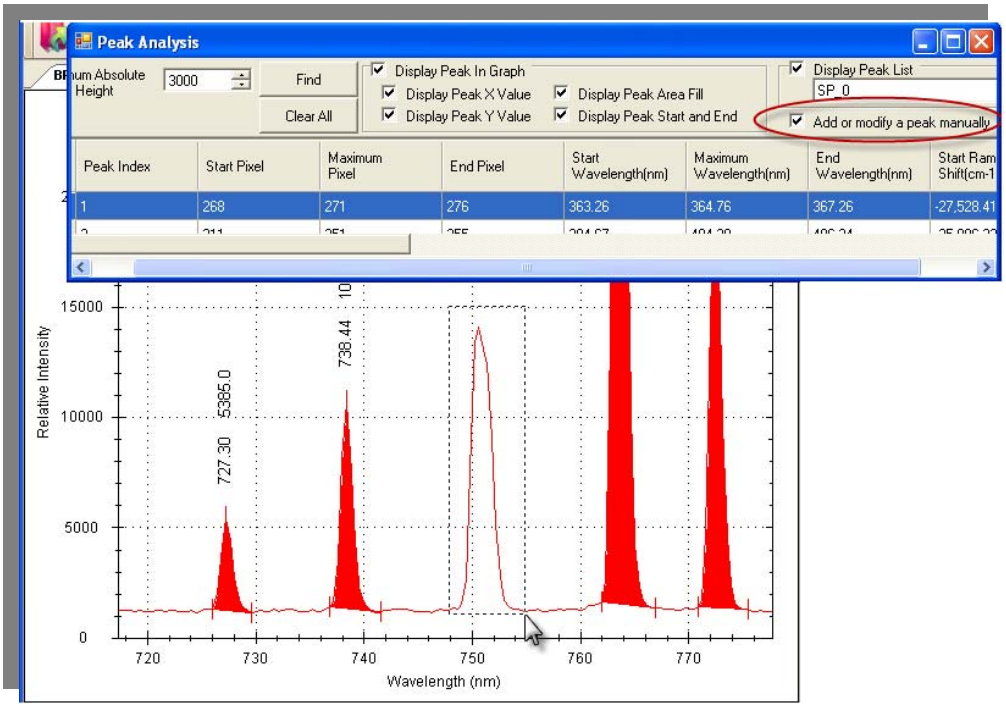
6.2.3. Add a Peak Manually

Check the box for **Add or modify a peak manually**. Place cursor on the peak you want to add, hold down the left button of the mouse and drag a dotted line around the peak. The boxed peak will be added to the list after the mouse button is releases.



6.2.4. Modify a Peak Manually

Check the box for **Add or modify a peak manually**, hold down left button of mouse to drag a dotted line box around the spectral feature that needs to be modified until you are satisfied with the change. Release the mouse for the modification result to be displayed.

6.2.5. Report

Point cursor to a “Peak Index**”** and activate this line, right click you mouse and select “Export Result” at popup menu, you can view a print preview of the report.

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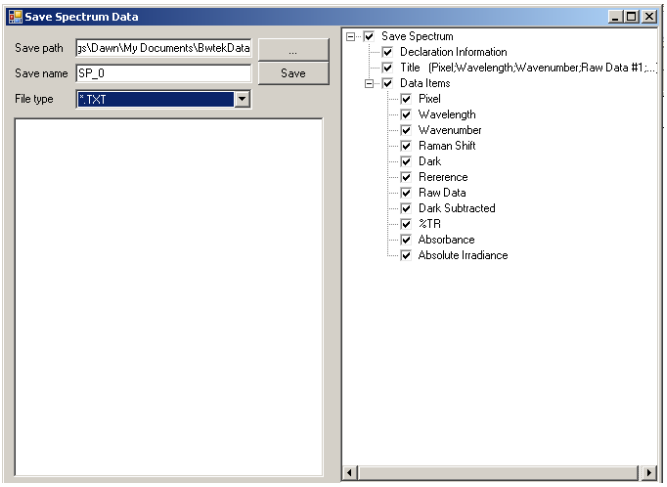
7. Save and Import Spectrum

7.1. Save A Single Spectrum

From the menu bar, click **File → Save A Single Spectrum**, or click on the tool bar to save the spectrum. A Save Spectrum window will show where user can select path, name, file type, as well as the data format related choices.



Here is another tip for you to save: place cursor on the spectrum name that you wish to save in **Spectra List Panel**, right click your mouse and select **Save This Spectrum** to save.

7.2. Save All Spectra Into ZIP file

From the menu bar, click **File → Save All Spectra Into ZIP File** to save all of the displayed spectra as a zip file. The saved spectra will show up in the graph area once you open this file.

7.3. Save All spectra To One File Folder

From menu bar, click **File → Save All Spectra To One File Folder** to save all spectra into a specified file folder, where each spectrum will be saved as a single file. These files will be named as SP_0.txt; SP_1.txt; …, SP_4.txt; … etc.

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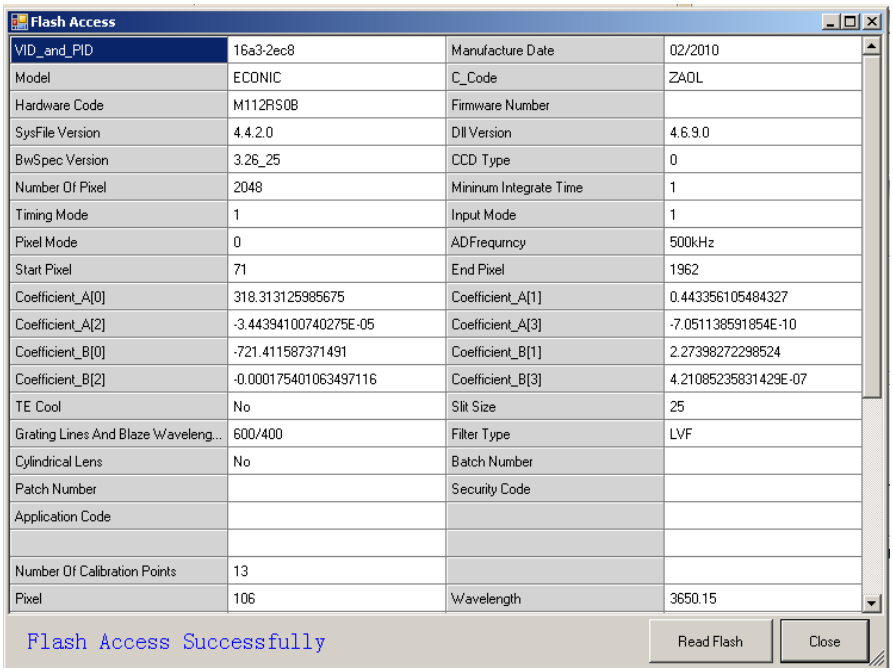
Select the path you would like to save these files into by clicking **Save path**, then click **Save** to finish.

7.4. Import Spectrum

From menu bar, click **File** → **Open Spectrum, or** click to open a previously saved spectrum into the graph area. Choose the file type and file you want to open and click **Open** to finish.

8. Read Flash

From the menu bar, click **Setup** → **Flash Access**, a dialog box will be displayed for the currently connected spectrometer info and settings. Click **Read Flash** at the bottom to restore parameter settings (integration time, multiplier, etc.) to the BWSpec 4 default setting as saved in the flash.


Flash Access
VID_and_PID 16a3-2ec8 Manufacture Date 02/2010
Model ECONIC C_Code ZAOL
Hardware Code M112RS0B Firmware Number
SysFile Version 4.4.2.0 Dll Version 4.6.9.0
BwSpec Version 3.26_25 CCD Type 0
Number Of Pixel 2048 Mininum Integrate Time 1
Timing Mode 1 Input Mode 1
Pixel Mode 0 ADFrequrncy 500kHz
Start Pixel 71 End Pixel 1962
Coefficient_A[0] 318.313125985675 Coefficient_A[1] 0.443356105484327
Coefficient_A[2] -3.44394100740275E-05 Coefficient_A[3] -7.051138591854E-10
Coefficient_B[0] -721.411587371491 Coefficient_B[1] 2.27398272298524
Coefficient_B[2] -0.000175401063497116 Coefficient_B[3] 4.21085235831429E-07
TE Cool No Slit Size 25
Grating Lines And Blaze Waveleng... 600/400 Filter Type LVF
Cylindrical Lens No Batch Number
Patch Number Security Code
Application Code
Number Of Calibration Points 13
Pixel 106 Wavelength 3650.15
Flash Access Successfully
Read Flash
Close

9. Plug-in

From the menu bar, click **Plug-In** →**Plug-in Manager** to enable or disable functions by selecting or deselecting function modules. Click **OK** to finish.

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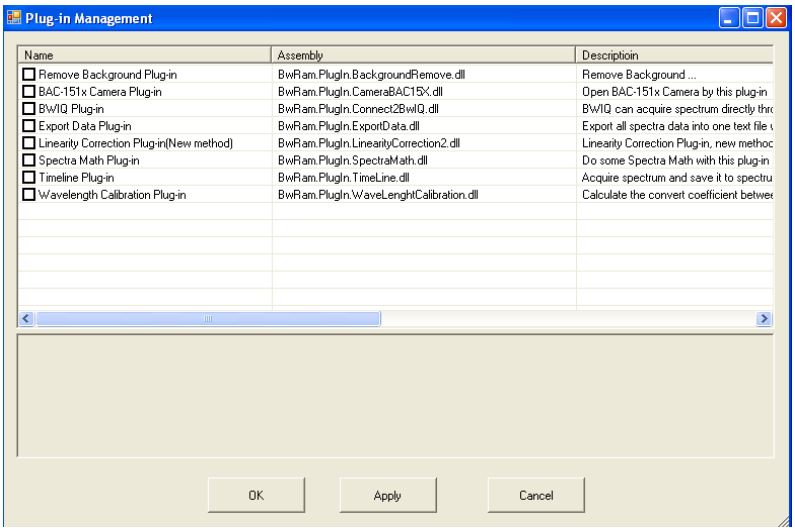

The selected Plug-In functions will be available and shown under **Tools** and **Option**.

9.1. Background Removal

The **Background Removal** function is to remove spectrum background (or to perform baseline correction).

Click **Tools** and select **Background Removal**. A display window with three spectra will be displayed: raw spectrum, automatically fitted background curve, and the spectrum after background removal. Lambda factor can be adjusted for manipulating the auto fitted background so as to achieve the desired background removal result. Click **Do** to apply changes.

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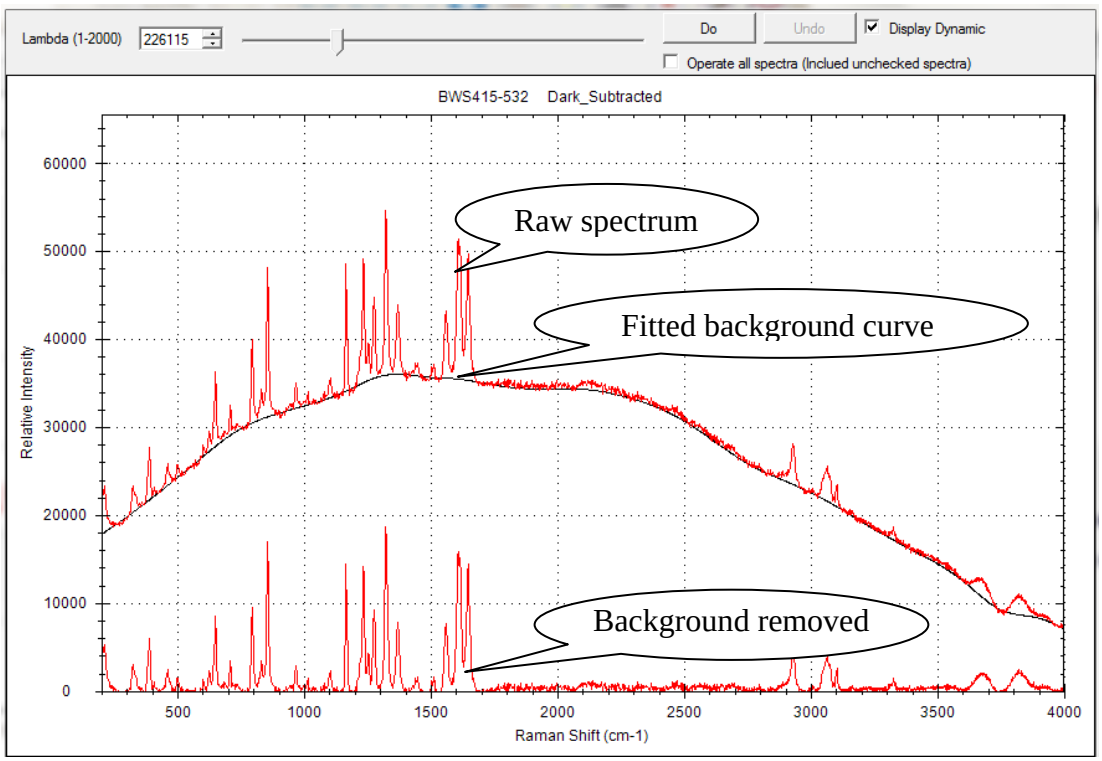

9.2. Export Data

Click **Tools** from the menu. Choose **Export Data→ Export All Spectra Data**, a dialog box will show up. Select the data information you want to export, click **Save as** button. All spectra data will be exported and saved into a text file.

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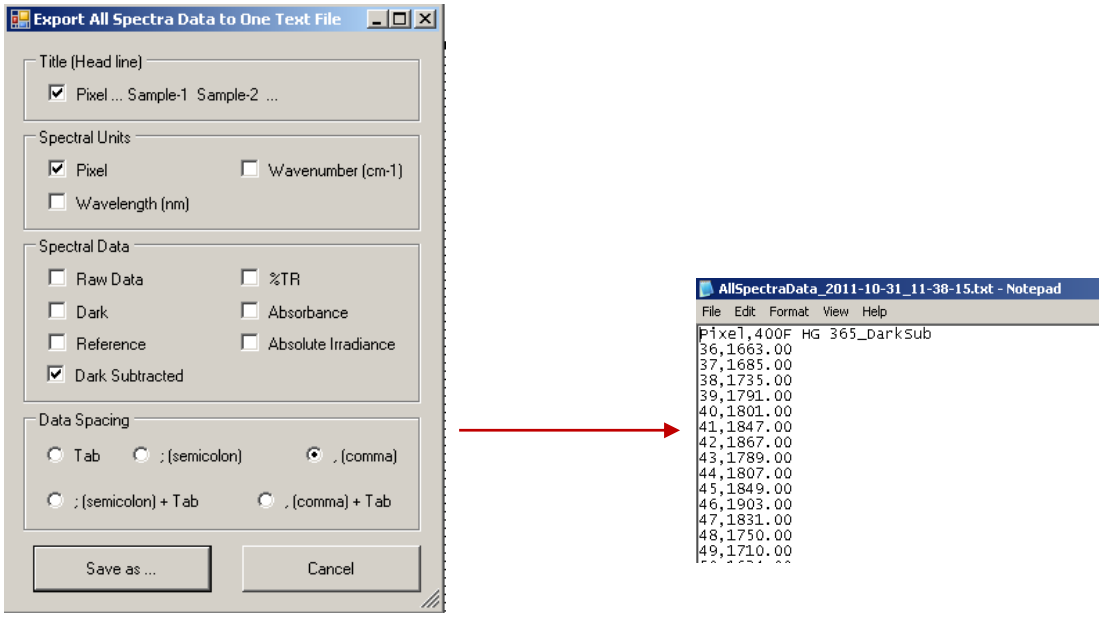

9.3. Derivative

Click **Tools** Derivative, next click, a dialogue box will appear for spectral derivative function options. Three derivative methods are provided for possible data pretreatment use:

- Point Diff:
- Savitzky-Golay
- Differential:

Select the desired derivative method, check Apply Derivative box to apply the derivative calculation to the currently active spectrum.

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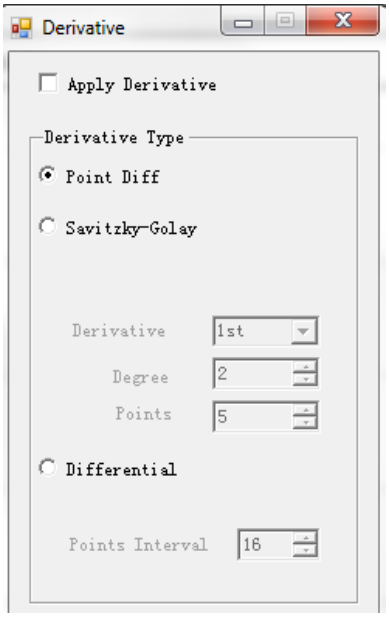

9.4. Timeline

Timeline function provides automated, timed recording of spectra according to the scheduled time interval settings with acquired spectrum at the time specified and saved into individual files.

9.4.1. Timeline (Equal Integration Time)

Click **Tools→Timeline→Timeline (Equal Integration Time**), a dialogue box will appear. Before starting timeline scan, you need to enter the settings in this box, including interval time, number of scans, file name prefix, file name postfix, and save path. Click button to start timeline scan. The spectra collected will be saved in the designated path. If no specific suffix is assigned, default _1, _2… will be assigned to each spectrum.

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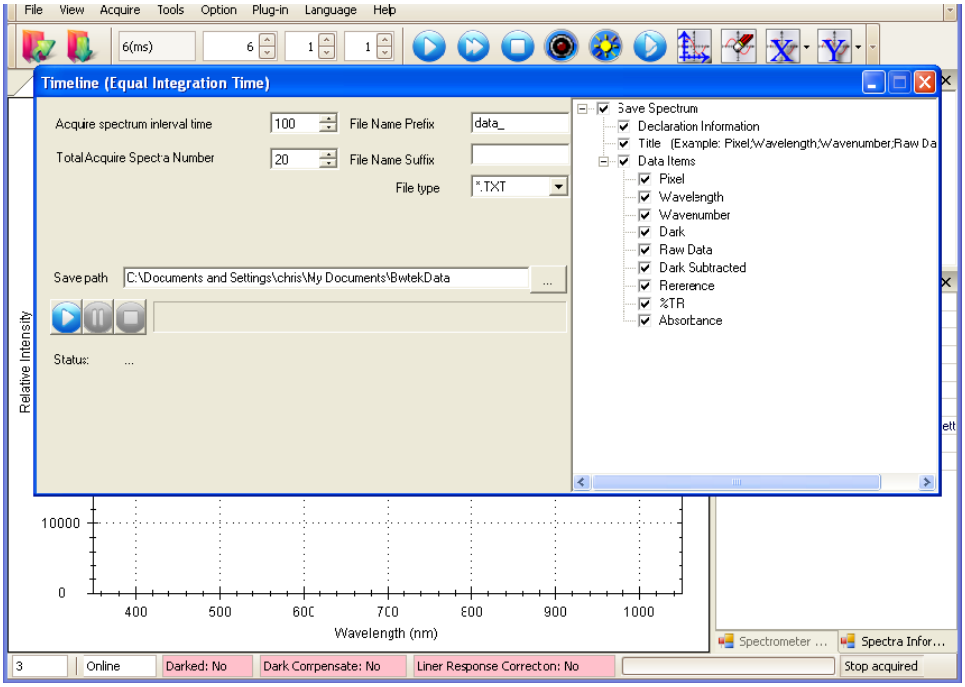

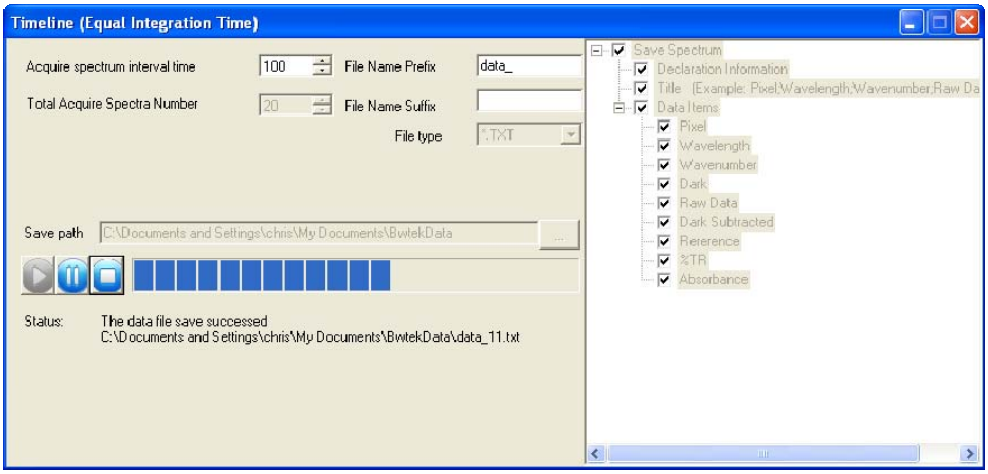

9.4.2. Timeline (Gradient Integration Time)

Click **Tools** and select **Timeline**, next click **Timeline (Gradient Integration Time)**, a dialogue box will appear.

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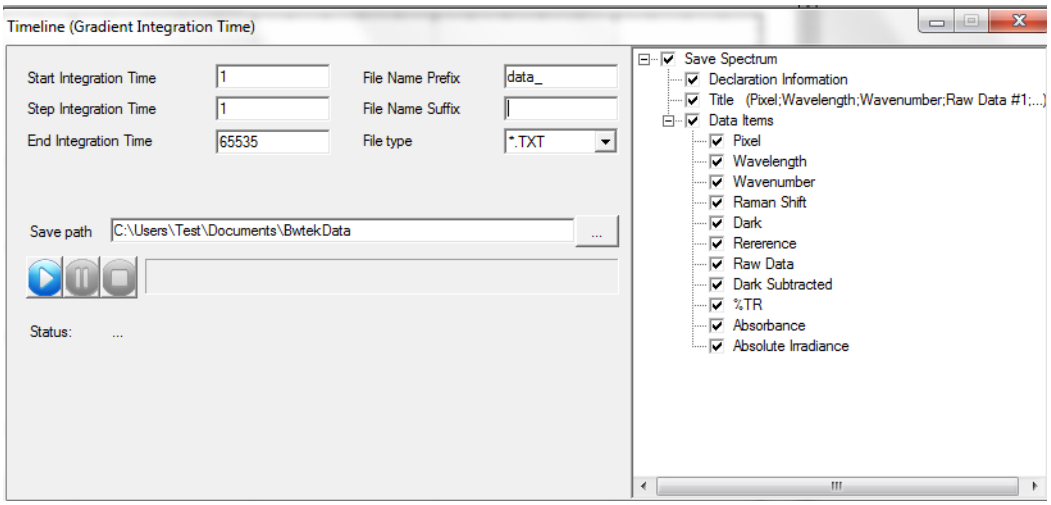
With gradient integration time, the integration time will change automatically according to the setting. When you finish one time acquisition, the integration time will automatically plus a step time on your last integration time, which will then be you next acquisition integration time. You can input step time in the dialogue box below. After each scan, the integration time will plus this step time as your next acquisition integration time to be used.



9.4.3. Timeline Load

To automatically load the files that were saved previously, click **Tools** and select **Timeline → Timeline load**, click load path to select the folder location of the timeline data while the corresponding files are displayed on the Spectrum display panel.

- Click button to automatically load each and every data file one by one.
- Click button to manually load the spectrum file forward, one at a time.
- Click button to manually load the spectrum file backwards, one at a time.
- Click button to resize the Timeline Load window.

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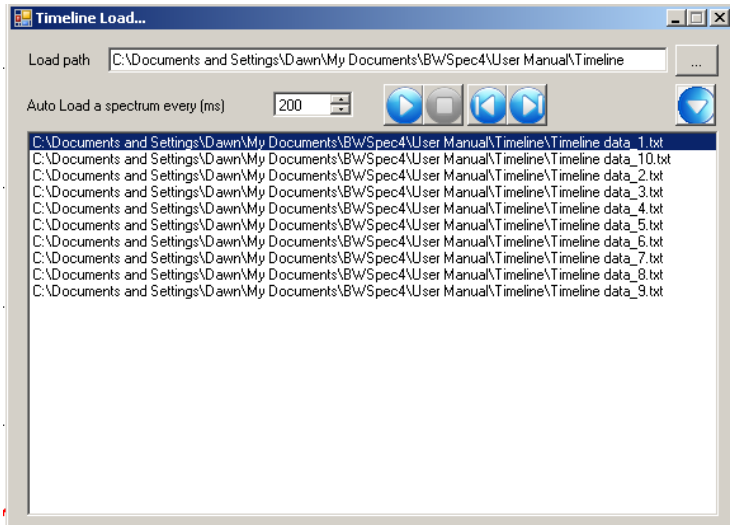
Timeline Load...
Load path
C:\Documents and Settings\Dawn\My Documents\BWSpec4\User Manual\Timeline
...
Auto Load a spectrum every (ms)
200
C:\Documents and Settings\Dawn\My Documents\BWSpec4\User Manual\Timeline\Timeline data_1.txt
C:\Documents and Settings\Dawn\My Documents\BWSpec4\User Manual\Timeline\Timeline data_10.txt
C:\Documents and Settings\Dawn\My Documents\BWSpec4\User Manual\Timeline\Timeline data_2.txt
C:\Documents and Settings\Dawn\My Documents\BWSpec4\User Manual\Timeline\Timeline data_3.txt
C:\Documents and Settings\Dawn\My Documents\BWSpec4\User Manual\Timeline\Timeline data_4.txt
C:\Documents and Settings\Dawn\My Documents\BWSpec4\User Manual\Timeline\Timeline data_5.txt
C:\Documents and Settings\Dawn\My Documents\BWSpec4\User Manual\Timeline\Timeline data_6.txt
C:\Documents and Settings\Dawn\My Documents\BWSpec4\User Manual\Timeline\Timeline data_7.txt
C:\Documents and Settings\Dawn\My Documents\BWSpec4\User Manual\Timeline\Timeline data_8.txt
C:\Documents and Settings\Dawn\My Documents\BWSpec4\User Manual\Timeline\Timeline data_9.txt

9.5. Linearity Correction

9.5.1. About Linearity Correction

Linearity correction will adjust the detector array's non-linear response to follow a calculated linear relationship against received detector photons using the calibration function obtained through a linearity calibration correction.

For example a typical detector array exhibits nonlinear response with respect to incident photons especially at low light level as well as close to the saturations. In these regions doubling photons or doubling detector exposure time will no longer result in two times the detector's output deviating from a desired linear response range.

NOTE: The "Linearity Correction" must be conducted by the factory in order for the calibration information to be saved into device memory; a copy will be recorded at the factory. "Linearity Correction" is an upgrade option item to be ordered at the same time of the spectrometer purchase

9.5.2. How to Conduct a Linearity Correction

For advanced users the linearity correction may be conducted at the customer site. From the menu bar, **Option→Linearity Correction**. The linearity correction window will appear.

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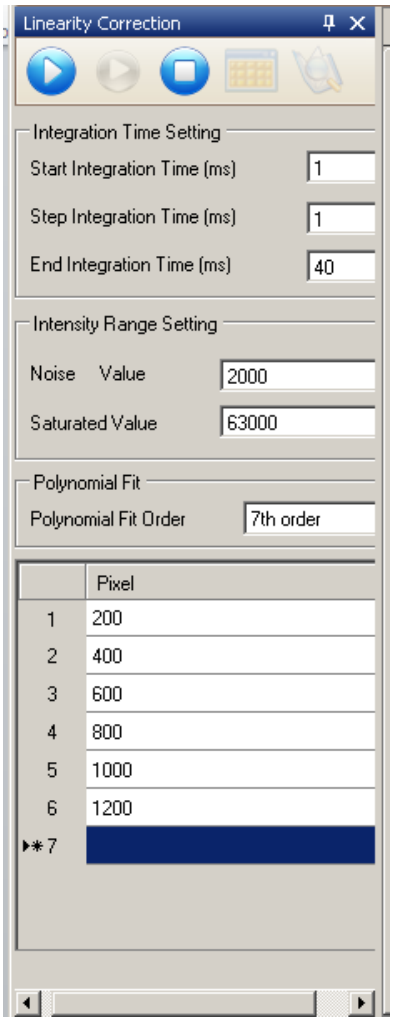

- Set the parameters for linearity correction on the screen.
- Press to start collecting the scans needed for linearity correction.
- Press to collect a dark scan with light off.
- Press to calculate linearity correction coefficients.

The Linearity Coefficients will be displayed on the top of the window along with a message:

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The linearity correction coefficients have been saved to para.ini file [YAXIS_CORRECTION] section.

NOTE: Make a backup copy of the parameter file with the new Linearity Coefficients that have been written to them for future reference. Once the Flash is reread the Linearity Coefficients will be lost. If you save a copy of the parameter file with the Linearity Coefficients already saved on it, you may Import this parameter file into the BWSpec software when needed.

NOTE: The key for a successful linearity correction calibration setup is to provide an adjustable intensity light input into the spectrometer to be calibrated so that the spectrometer shows a light response 500-1000 counts above its dark levels at its shortest integration time. This will provide the calibration with maximum useable calibration dynamic ranges.

9.5.3. Activate Linearity Correction

To activate linearity correction, from the menu bar **Option → Enable /Disable Linearity Correction**.

9.6. Relative Intensity Correction

9.6.1. About Relative Intensity Correction

Relative intensity correction is specific for Raman spectrometer users. Its purpose is to correct individual spectrometer's unique relative spectral responses against a traceable standard. The corrected spectral response of a Raman spectrometer makes it possible for meaningful comparisons between data obtained from different instruments. The calibrated spectral response also reveals quantitative vibrational intensity information between different Raman features within a given Raman spectrum.

The relative intensity correction involves the use of Standard Reference Material 2241 (SRM 2241) for Raman spectrometers where a 785nm excitation laser source is used, and SRM2242 where a 532nm excitation laser source is used.

9.6.2. How to conduct a relative intensity correction

This calibration is an option a customer may order at the time of purchase. For advanced users this may be conducted at a customer site with appropriate equipment.

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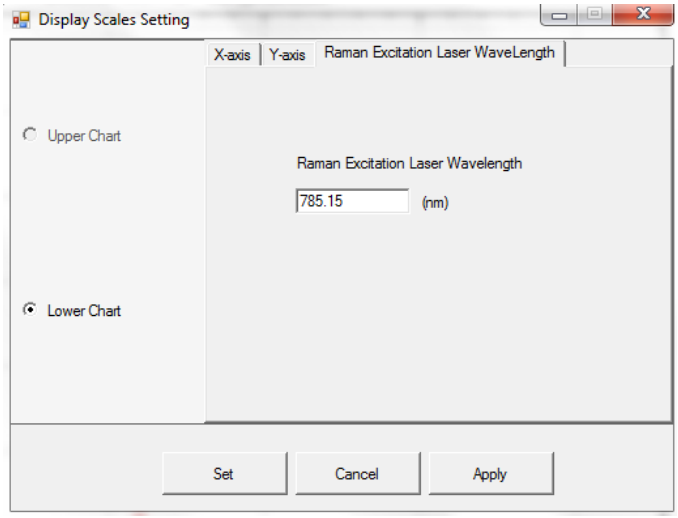
You must have a Probe connected to a Raman system or a Laser and a spectrometer in order to get proper results.

- Make sure that the wavelength of the excitation laser you are using is entered into the **Raman Excitation Laser Wavelength** page on the **Display Scales**, for example, 785nm.



- Determine the appropriate integration time: use the standard reference material SRM2241 (for 785nm) or SRM2242 (for 532nm) to run a scan. The integration time of the scan should be adjusted to the value so that the highest intensity level is just below saturation level (65000 counts).
- Run a dark scan with the same integration time. For B&W Tek Raman system the laser turns off automatically when dark scan is collected. For modular Raman spectrometer, make sure the laser is off when a dark scan is collected.
- Run a reference scan using SRM2241 (or SRM2242) with the same integration time, with laser being turned on.

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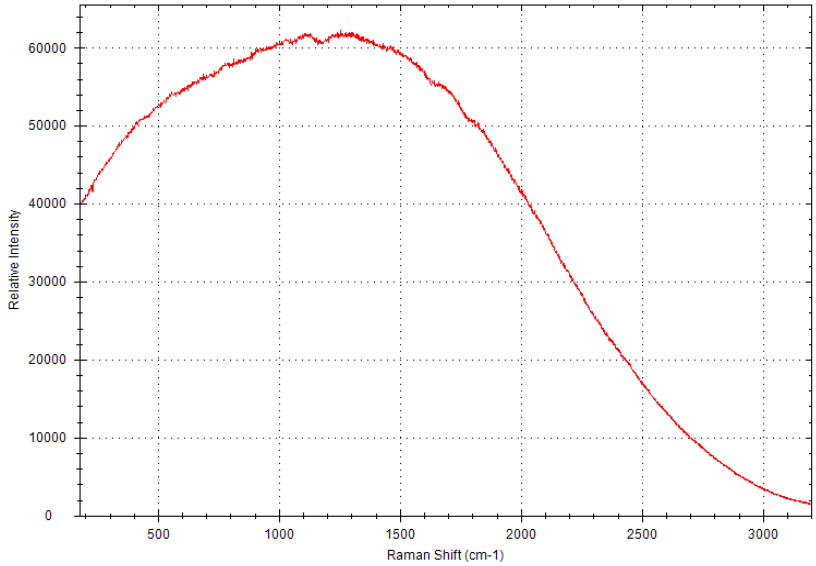
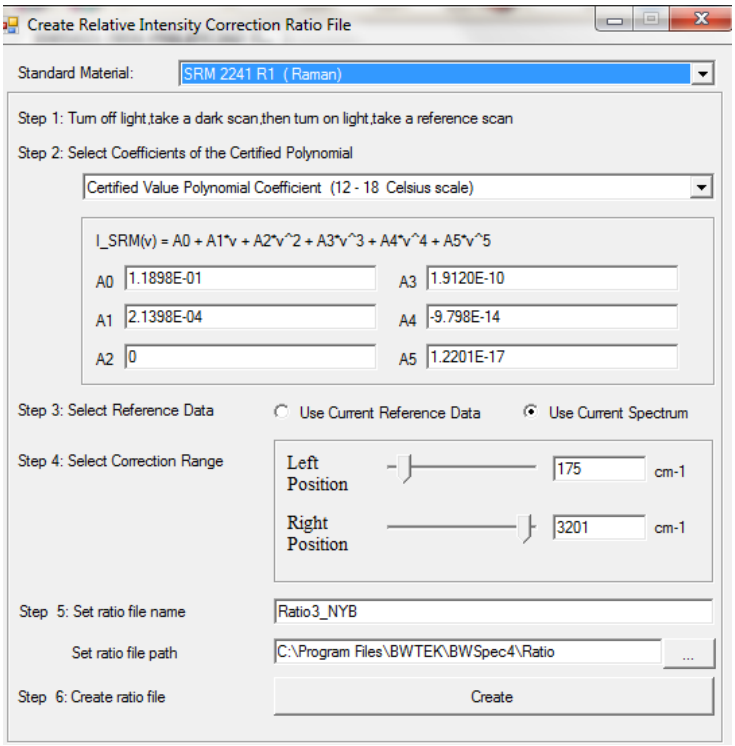


- From the menu bar, **Option → Relative Intensity Correction**. The Relative Intensity Correction window will appear.



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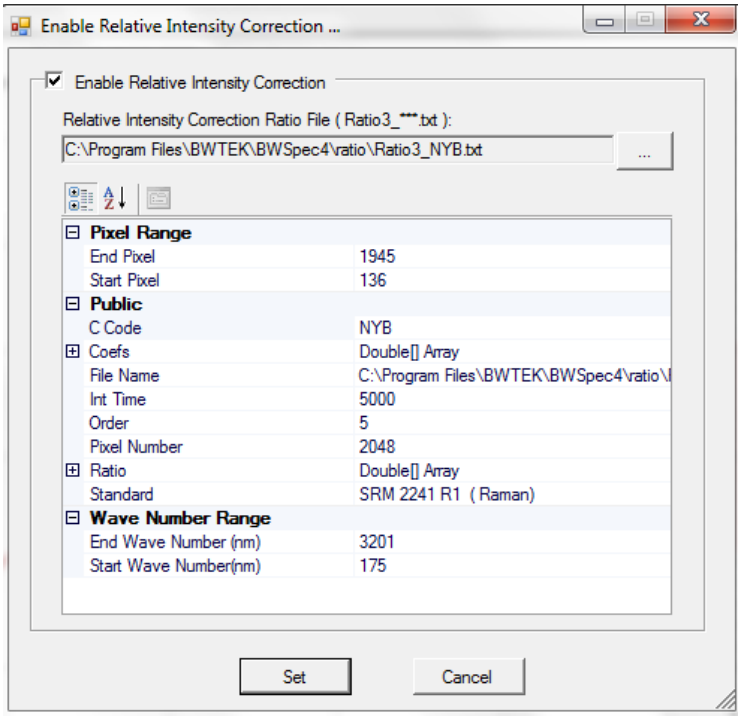
- Select appropriate standard material (for example, SRM2241)
- Select “Use Current Spectrum”
- Enter correction range (left position, right position)
- Set the ratio file name and the path where the ratio file will be stored.
- Click **Create** button. The Relative Intensity Correction file is created and the Ratio3 file is saved in the designated path.

9.6.3. Apply Relative Intensity Correction

To turn on relative intensity correction feature, from the menu bar **Option → Enable /Disable Relative Intensity Correction**. Check the box “Enable Relative Intensity Correction”, and click on ... to locate the Ratio3 file specific to the system calibrated with. Click **Set** to apply.



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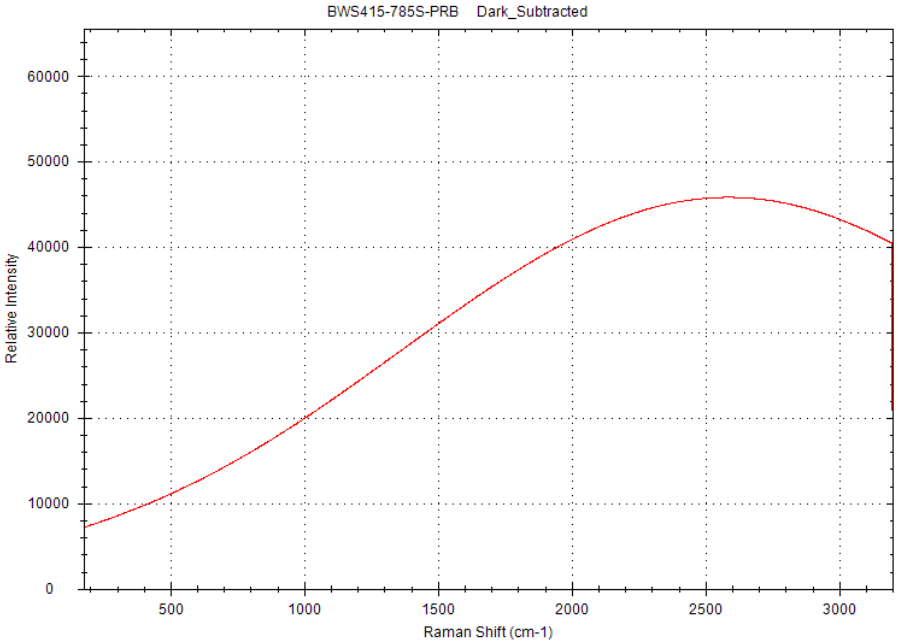

9.7. Reference Materials Correction

9.7.1. About Reference Material Correction

In applications such as in diffused reflectance measurements, a certified reflectance standard is often used to serve as a reference. The %R values throughout the measurement range are then calculated by using ratios with respect to the reference in a relative sense. With the available certified %R values the BWSpec software can calculate the “absolute reflectance” against the reference.

The following is a table of a typical certified PTFE type material spectral reflectance white diffuse reflectance standard (SRS-99-010)

Wavelength (nm)	Certified %R value		Wavelength (nm)	Certified %R value
360	98.5		600	98.9
370	98.7		610	98.9
380	98.7		620	98.9
390	98.7		630	98.9
400	98.8		640	98.9
410	98.8		650	98.9

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420	98.8		660	98.9
430	98.8		670	98.9
440	98.8		680	98.9
450	98.8		690	98.9
460	98.8		700	99.0
470	98.8		710	98.9
480	98.9		720	99.0
490	98.9		730	98.9
500	98.9		740	98.9
510	98.9		750	99.0
520	98.9		760	98.8
530	98.9		770	98.9
540	98.9		780	98.9
550	98.9		790	98.9
560	98.9		800	99.0
570	98.9		810	98.9
580	98.9		820	99.0
590	98.9		830	98.9

If we define %Rs (non-correction) as the sample percent reflectance at a given wavelength:

%Rs (non-correction) = (Sample intensity/Reference intensity)*100

After reference material correction:

%Rs (absolute) = %Rs(non-correction) * Certified %R value/100

where all values are calculated at given wavelengths across the calibrate wavelength range.

9.7.2. Generate Reference Material Correction Ratio File

This section is for advanced users only.

- Collect a spectrum using reference materials.
- Select **Option→ Reference Material Collection**.
- Click to browse to locate the “Reference Material ratio.txt” file. You will be directed to the default path where this file is stored at: C:\Program Files\BWTEK\BWSpec4\ratio\. This file contains the certified values of spectral

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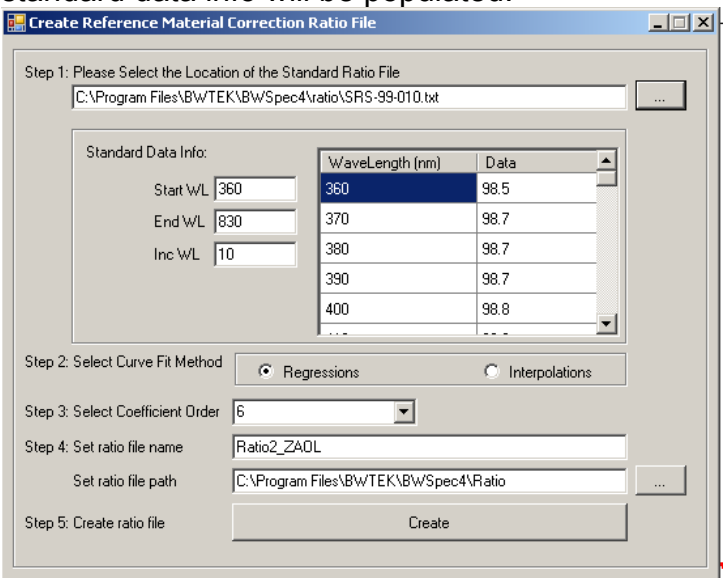
reflectance over the interested wavelength range. After the file is loaded, the standard data info will be populated.



- Follow the steps stated to fill out the parameters for the correction. The default ratio file name is Ratio2_spectrometer-code.
- Clock **Create** to generate Ratio2 file.

9.7.3. Enable Reference Material Correction Files

- Select **Option→ Enable Reference Material Correction**.
- Check on box “Enable Reference Material Correction”.
- Click ... to locate the “Reference Material correction ratio2.txt” file.
- Click **Set**.

9.8. Absolute Irradiance

9.8.1. About Irradiance Calibration

Irradiance Calibration can be conducted by BWTek, Inc. using NIST Traceable Standard Irradiance Standards and calibration setups, if so desired. Irradiance Calibration is an option that can be ordered at the time of placing a spectrometer purchase. Before activating your Irradiance Calibrated unit, using the accompanied calibration file, Linearity Correction should be performed first.

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9.8.2. How to Conduct Irradiance Calibration

This section is for advanced users only.

In order to conduct Irradiance Calibration, you must first have a NIST Traceable Lamp Source with Certified Values which cover the spectral range you will be calibrating your spectrometer to and .DAT file that will have accompanied your lamp.

Another factor is having the correct input optics for your spectrometer to collect the light such as a fiber and Collimating Lens, as an example.

The spectral irradiance calibration will allow a spectrometer to convert spectral measurements to absolute spectral irradiance measurements in units of light power in W, mW or µW / [cm^2*nm]. Alternatively, a spectral irradiance calibration can be used to calibrate the spectrometer for emissive photometric measurements, such as measurements of the color of an emissive source (for example, LED).

Your setup conditions, distance from source, and lamp current, must be as close as possible to what your NIST Certificate states in order to conduct a successful calibration process. Ideally, the light source should slightly under fill the spectrometer's angular aperture. The light source illuminates the spectrometer at a distance specified in the lamp source's calibration data.

Given the correct experimental setup the spectral irradiance calibration proceeds as follows with the assumption that the spectrometer is equipped with a suitable input optic and linearity correction:

- Adjust the integration time so that the maximum spectral response feature is just below the spectrometer saturation level against the certified lamp at a specified distance. Stop the acquisition and freeze all physical setup with minimal disturbance.

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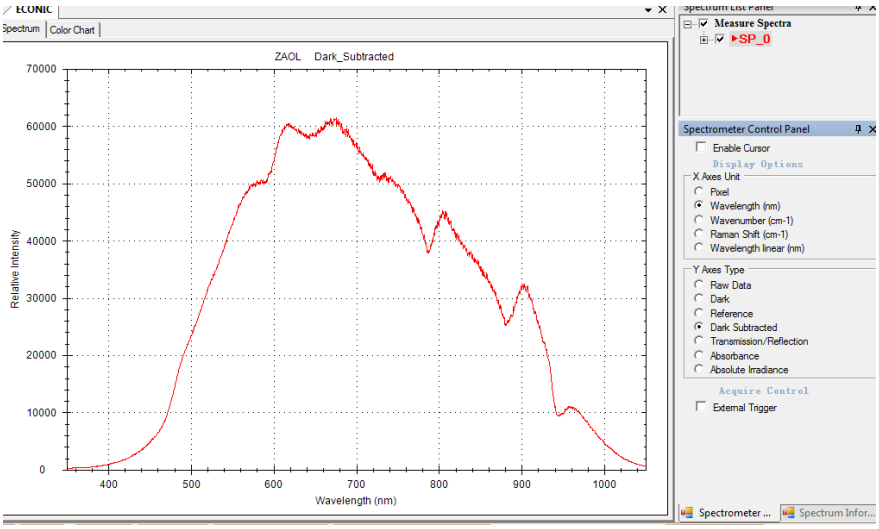
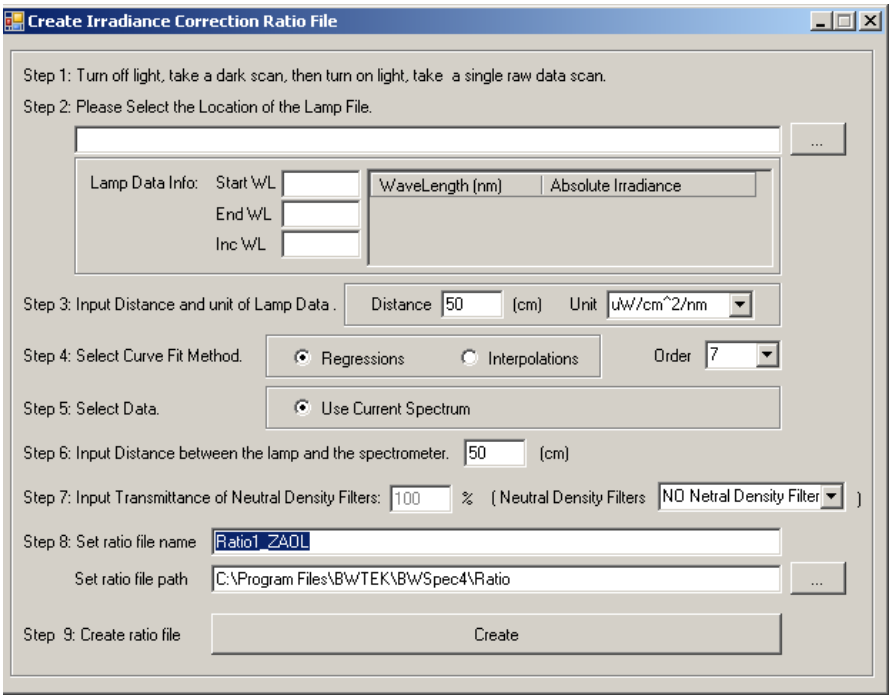


- Creation of Irradiance Ratio File:
  From the Menu Bar, select **Option** → **Irradiance Correction**. Follow the steps stated in the following window to proceed with irradiance calibration procedure.



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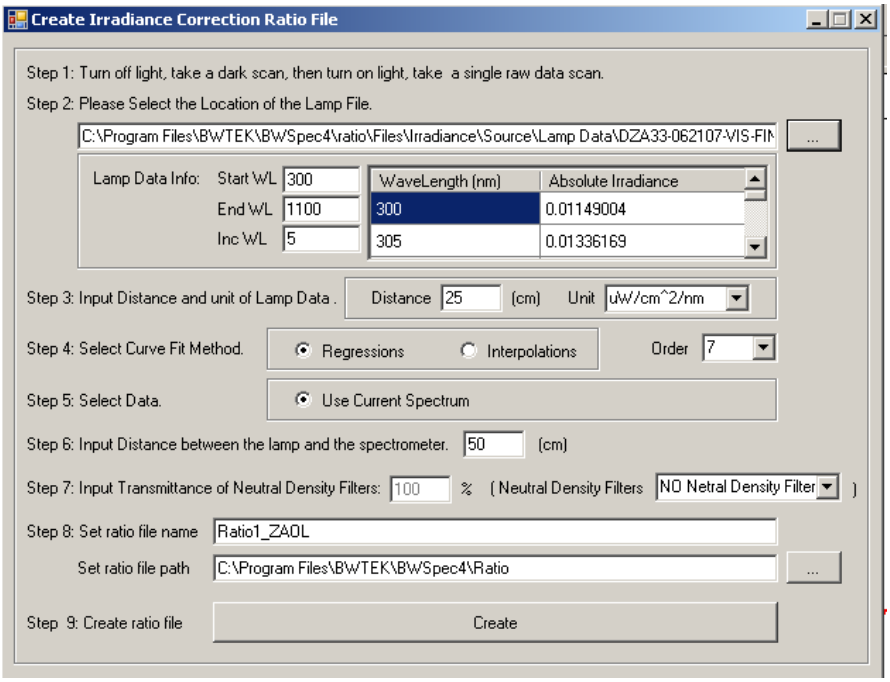
- Step 1: Turn off light, take a dark scan. Then turn on light, take a single raw data scan.
- Step 2: Click ... button and locate the lamp data file for the light source you are using for irradiance calibration. Your lamp data file must be configured in a manner in which BWSpec can read it. Please see the Appendix at the end of this manual section called “Definition of Irradiance Data File Format” for information on formatting. You can also view the file “D301.dat” for an example of format, which can be located in the folder where BWSpec is installed.


Create Irradiance Correction Ratio File
Step 1: Turn off light, take a dark scan, then turn on light, take a single raw data scan.
Step 2: Please Select the Location of the Lamp File.
C:\Program Files\BWTEK\BWSpec4\ratio\Files\Irradiance\Source\Lamp Data\DZA33-062107-VIS-FIN
Lamp Data Info:
Start WL 300
End WL 1100
Inc WL 5
WaveLength (nm)
Absolute Irradiance
300
0.01149004
305
0.01336169
Step 3: Input Distance and unit of Lamp Data .
Distance 25 (cm) Unit uW/cm^2/nm
Step 4: Select Curve Fit Method.
Regressions
Interpolations
Order 7
Step 5: Select Data.
Use Current Spectrum
Step 6: Input Distance between the lamp and the spectrometer. 50 (cm)
Step 7: Input Transmittance of Neutral Density Filters: 100 % (Neutral Density Filters NO Netral Density Filter)
Step 8: Set ratio file name Ratio1_ZA0L
Set ratio file path C:\Program Files\BWTEK\BWSpec4\Ratio
Step 9: Create ratio file
Create

- Step 3: Input the distance for your NIST Calibrated Light Source, at which it was calibrated. This information will be contained on your Certificate or the .DAT file.
- Step 4: Coefficient Order, used for Curve Fit, default value 7.
- Step 5: Select which spectrum to use for your Reference Data. If you’ve already taken a “Reference Scan”, select “Use Current Reference Data”
- Step 6: Select the distance that you have setup between your input optic and your certified light source. Also make sure to enter into the dialog box all calibration related information such as the additional optics used, etc.. Be careful to select correct units to match the certified data provided as in the reference certified lamp data file.

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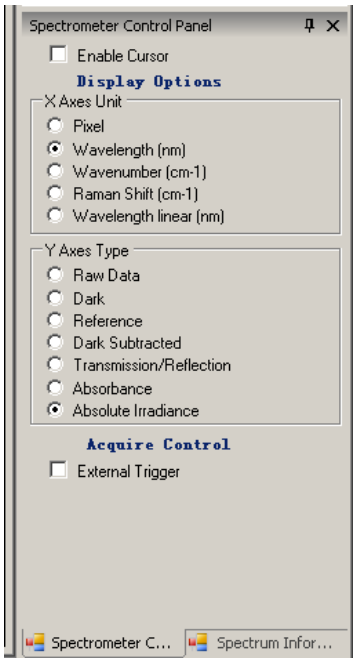
- Step 7: Input transmittance of neutral density filters
- Step 8: Name the ratio File in which you would like it to be saved as. We suggest your keep the default naming scheme, “Ratio1_C-code” of the spectrometer. Save Path: Location to where the ratio file will be saved to.
- Step 8: Click **Create** to generate the “Irradiance Ratio File”

9.8.3. Apply Irradiance Ratio File

- Select **Option→ Enable /Disable Irradiance Correction**
- Check on box “Enable Irradiance Correction”.
- Click to locate the irradiance correction “Ratio1.txt” file.
- Click **Set**.
- Click “Absolute Irradiance” on the Spectrometer Control Panel. The Absolute Irradiance curve will show on the display.



You may need to adjust the X-axis and Y-axis scales in order to get the suitable display scale settings.

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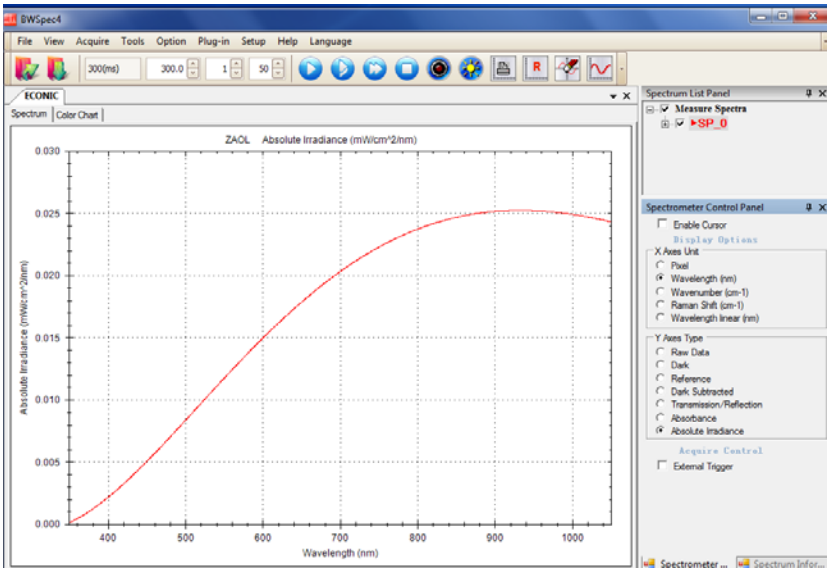

9.9. Color Measurement

9.9.1. About Color Measurement

The color measurement is to characterize an object (for example, illumination source) in terms of its chromaticity and radiometry. Chromaticity refers to the quality of the object regardless of its luminance, while radiometry measures the radiant energy or electromagnetic energy of the object.

The color measurement result shown in the “Color Chart” tab will only be made available when the spectrometer in use covers from at least 400 nm through no shorter than 700 nm spectral range.

Before performing a color measurement, the system should be normalized or irradiance calibrated.

From the menu bar, select **Setup** → **Color Setup**. A dialog box will display, where the settings for color measurement can be adjusted.

- Inside the box for “**Color Calculation Source**”, a dropdown menu will allow user to choose between **%T/R** or **Irradiance** for the measurement.

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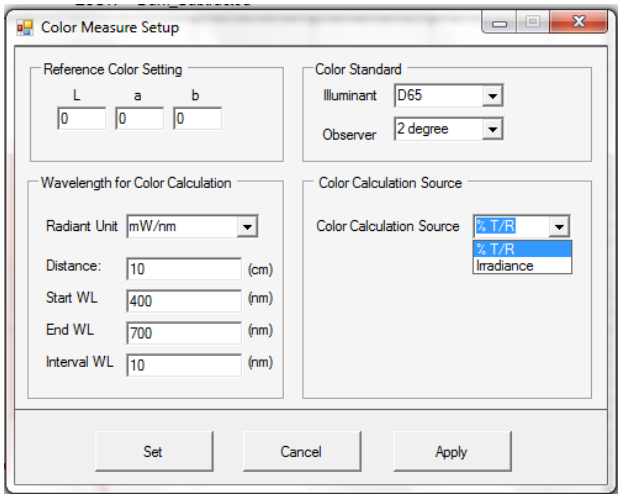
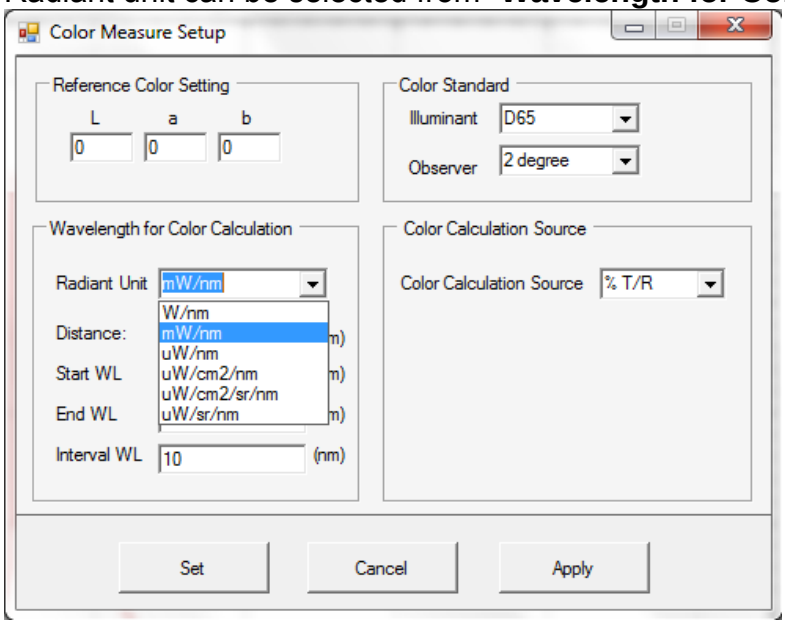


- Radiant unit can be selected from "**Wavelength for Color Calculation"** box:



- Select **Distance**, **Start WL**, **End WL**, and **Interval WL** for the measurement.
- Select color measurement standard from "**Color Standard"** box, including **Illuminant** and **Observer**.

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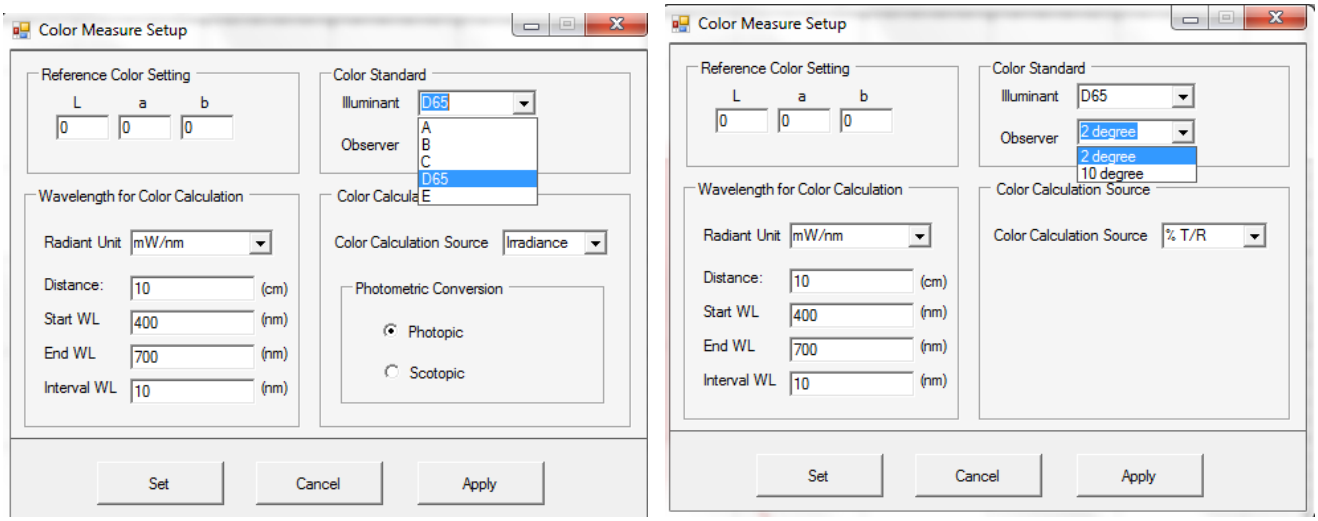
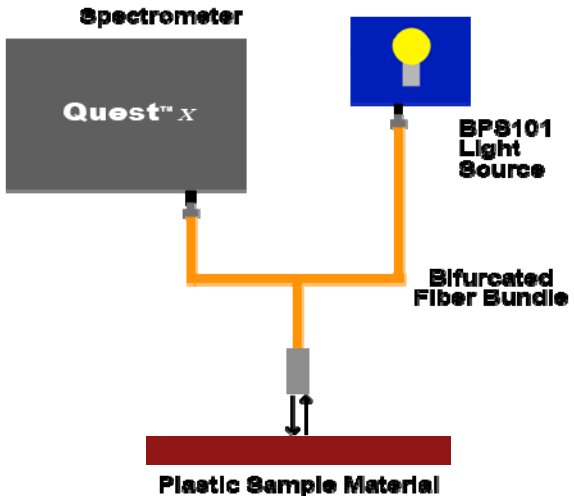


9.9.2. Reference and Dark Scan for %T/R Measurement

To perform a %T/R based color measurement, a white reflectance standard in reflectance setup and a stable light source covering the color range should be used. Light sources such as the BPS101, BPS120 from BWTek are suitable candidates.

As the apparent color of reflective objects depends upon both the spectral response of the spectrometer and the spectral output of the illumination source, a reflectance reference scan should be performed often so that the error due to the lamp drift is minimized.



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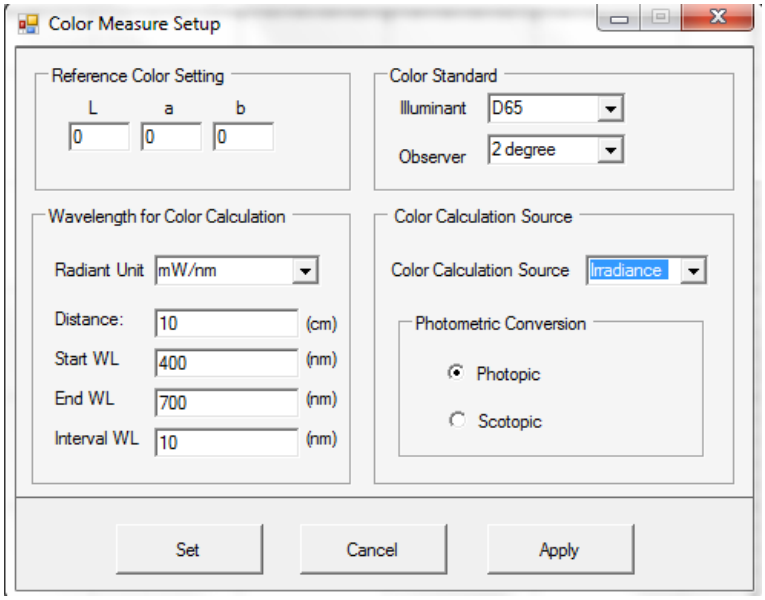
Connect the Light Source and the spectrometer via a fiber reflectance probe. Turn on the light source and allow it to warm up.

- Perform a Reference Scan
- Dark Scan using the same integration as the reference scan. Make sure to place the probe onto an absorbing black material or physically block the light from entering into the probe for dark scan.

9.9.3. Irradiance for Color Measurement

To perform irradiance calibration based color measurement:

- From the menu bar, select **Setup** → **Color Setup**. A dialog box will display, where the settings for color measurement can be adjusted. Inside the box for "Color Calculation Source", select **Irradiance** for the measurement.



- Enable irradiance calibration from Option → Enable /Disable Irradiance Correction, and select the corresponding irradiance correction ratio file (Ratio 1_***.txt).
- Calculate color perceived with the "Photopic" or "Scotopic".

9.9.4. Color Analysis

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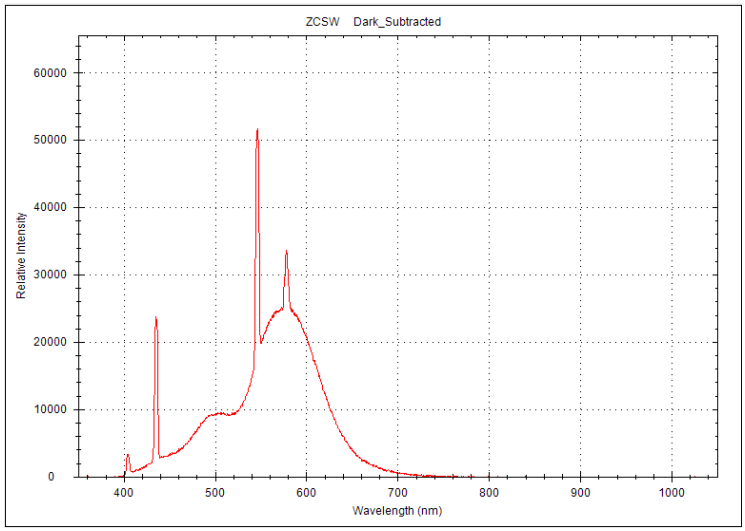
To acquire sample color data:

- Place the probe onto the desired sample to be measured.
- Acquire data scan on the sample material intended for color analysis.



9.9.5. Data Display

Click the "**Color Chart**" tab for chromaticity diagram and data display. Options of four different CIE color space are available:

- CIE xyY color space

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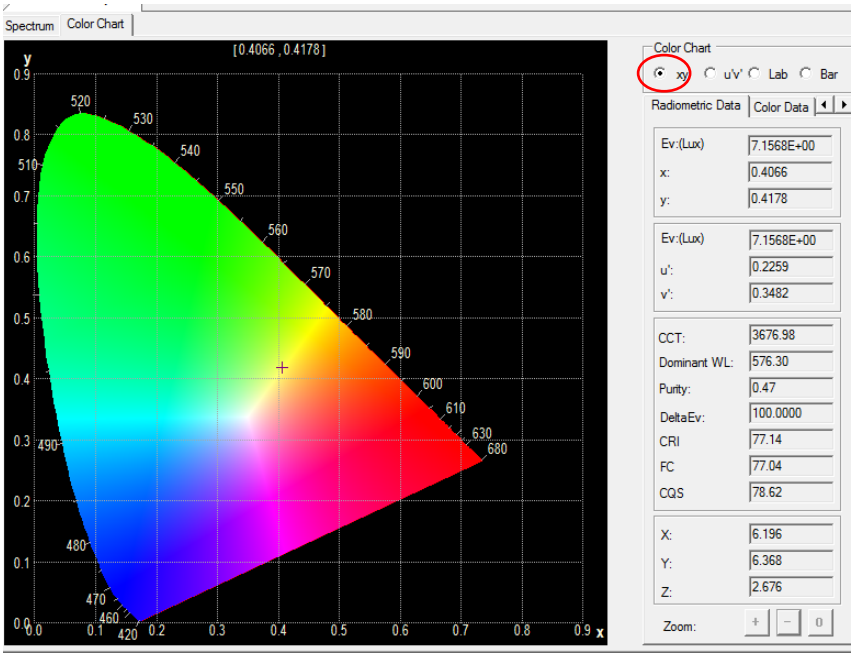
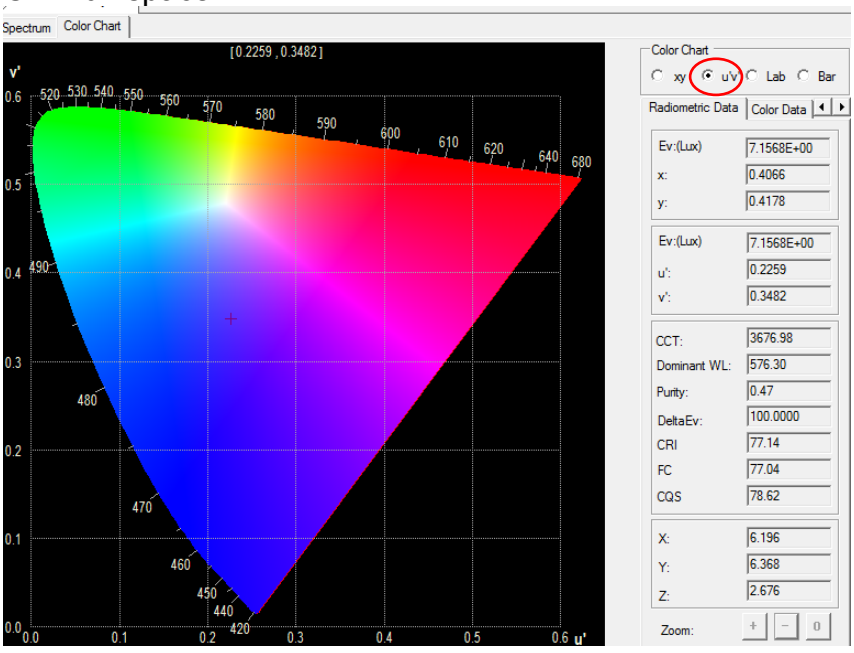


- CIE Luv space



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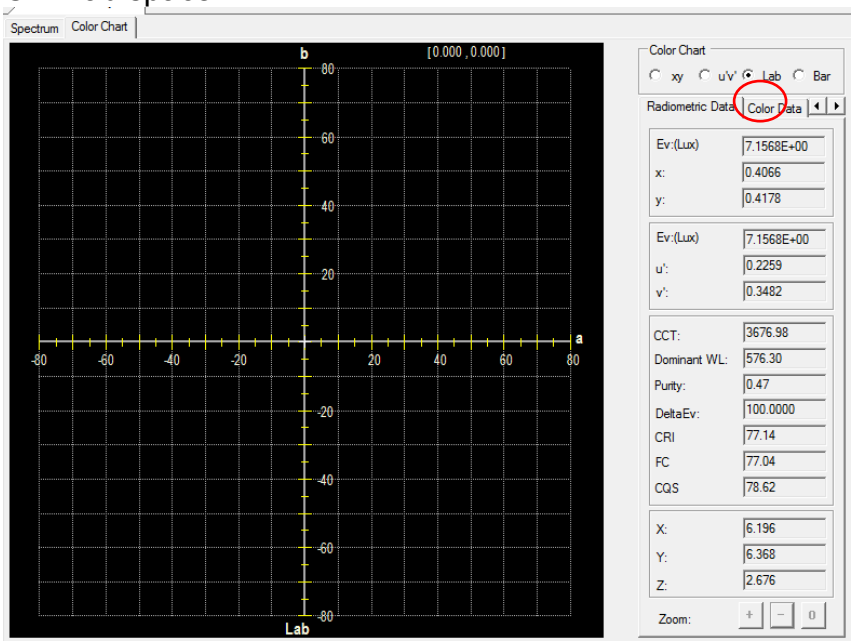
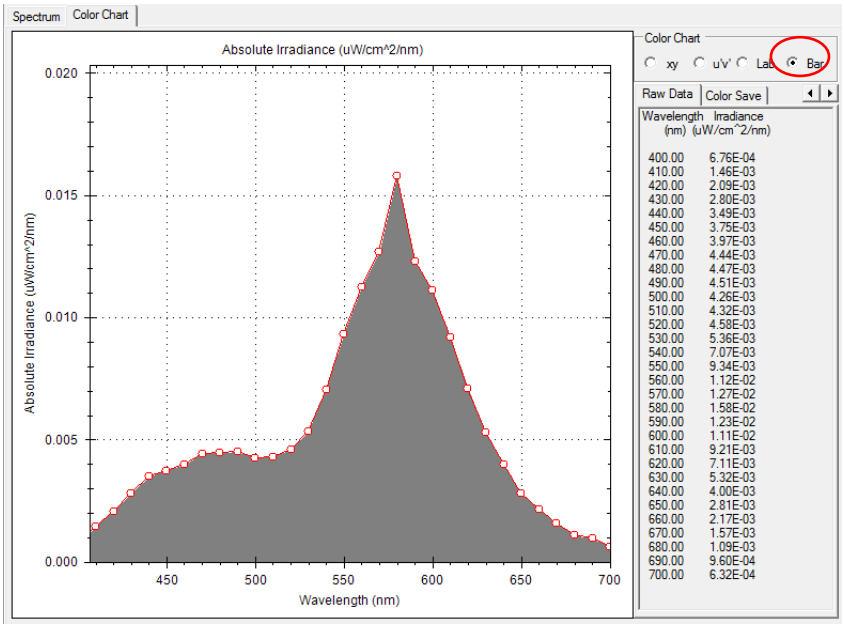
- CIE Lab space



- Color Bar



The radiometry and chromaticity data is displayed in five categories.

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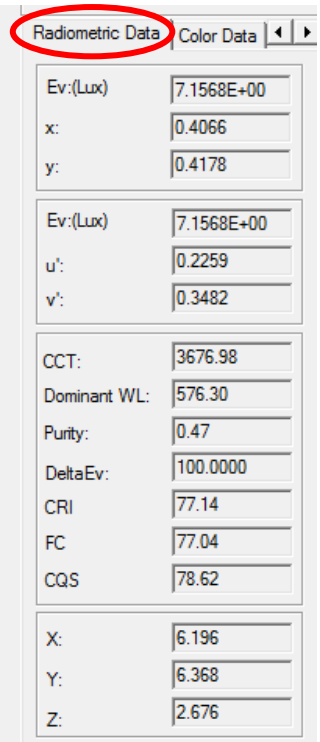
- Radiometric Data



- Color Data

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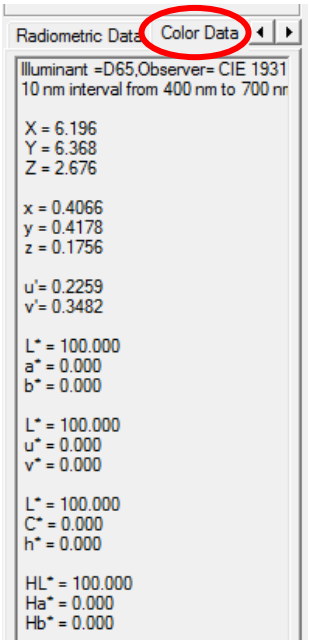
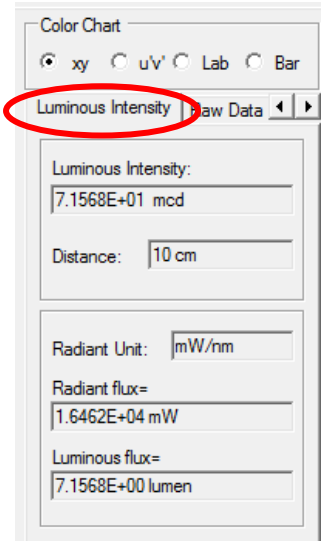


- Luminous Intensity



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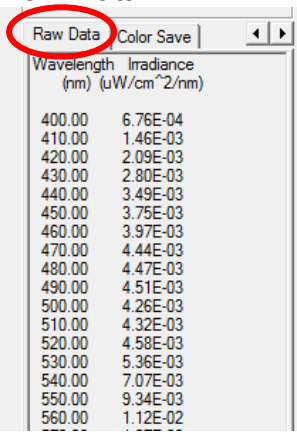
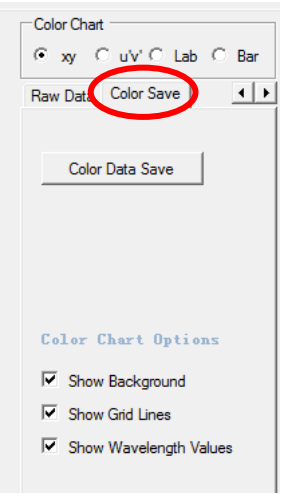
- Raw Data



- Color Save



Click **Color Data Save** to save the color data into BWSpec Color TXT file (.*txt)

There are three Color Chart Options available for color diagram setting:

- Show Background
- Show Grid Lines
- Show Wavelength Values

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Appendix A: Irradiance Ratio File Data Definition

Ratio.txt File details and explanation of data:

RATIO.TXT INFORMATION	EXPLANATION
BWSpec Version=BWSpec 3.26	Software Version
Ratio File Version=1.0	Ratio File Version
CCode=XXX	C-code of Unit
Int.Time=1100	Integration Time Data was acquired at for the Ratio File
Distance=75	Fiber to Light Source Distance used to create Ratio File
Lamp Name=350-780.DAT	Name of Lamp Data File Used
Lamp StartWL=350	Starting WL of Lamp Data File Used
Lamp EndWL=780	Ending WL of Lamp Data File Used
Lamp IncWL=10	Increments of WL pts from Start WL
Lamp Measure Distance=75	Distance Lamp Data file was created
Lamp Unit Index=2	Index 0 =W/cm^2/nm; Index 1 = mW/cm^2/nm; Index 2 = uW/cm^2/nm; Units will match the Lamp Data file and the units of the
Lamp Coefs Order=7	Order of curve fit
Coefs_C0=-102.802359649056	Curve Fit Values
Coefs_C1=1.38796702045458	Curve Fit Values
Coefs_C2=-0.00789398471358277	Curve Fit Values
Coefs_C3=2.45424259313939E-5	Curve Fit Values
Coefs_C4=-4.51571710685247E-8	Curve Fit Values
Coefs_C5=4.93405335866037E-11	Curve Fit Values
Coefs_C6=-2.9685358194907E-14	Curve Fit Values
Coefs_C7=7.588143959E-18	Curve Fit Values
irrands_yaxis_min=0	Y-axis minimum value, based on the start WL for the irradiance range
irrands_yaxis_max=4.38087481104945	Y-axis maximum value, based on irradiance WL range chosen
irrands_DispWLMin=350	Display Scales Settings
irrands_DispWLMax=780	Display Scales Settings
start_wv_irrands=350	Start WL for Irradiance Calibration (should match Lamp StartWL)

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end_wv_irrands=780	End WL for Irradiance Calibration (should match Lamp EndWL)
interval_wv_irrands=10	Increments of WL pts from Start WL to End WL (should match Lamp
Pixel ; Ratio	Pixel value ; Ratio (w/out Linearity Correction); Ratio (with Linearity Correction)
272;5.88055754188743E5;4.87368884634631E-5	
273;6.81553361643328E-5;5.60679388523222E-5	
274;7.19969136787624E-5;5.9194063207757E-5	
275;7.51481427041512E-5;6.17289907679508E-5	
276;6.89485036671211E-5;5.70395476167662E-5	
277;7.6339758550259E-5;6.28272853236966E-5	
278;7.85587836791279E-5;6.46321960184881E-5	
279;7.76122094106046E-5;6.39171821593676E-5	
280;7.9296241566551E-5;6.53590352790445E-5	

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Appendix B: Definition of Irradiance Data File Format

Example of a Certified Reference Lamp data file (ie. D300.DAT, Tungsten lamp)

Light Touch Software Data File
2.3a
0
TUNGSTEN 16V/6A
2020-31B W/Supp.Lens,NM-7DH 290-1110nm,DC-51C 200-1010nm,Silicon 200-1100nm

06-13-2003
14:38:16
RS-10A S/N:HL0191 IRRADIANCE

5	**---------- start flag**
350	**---------- wavelength start (nm)**
1100	**---------- wavelength end (nm)**
10	**---------- wavelength step (nm)**
4.762099E-02	**----------Irradiance of wavelength (350+0*10)= 350nm**
5.982313E-02	**----------Irradiance of wavelength (350+1*10)= 360nm**
7.276911E-02	**----------Irradiance of wavelength (350+2*10)= 370nm**
8.726646E-02	**----------Irradiance of wavelength (350+3*10)= 380nm**
0.1042587	**----------Irradiance of wavelength (350+4*10)= 390nm**
…..	
…..	
2.50559	**----------Irradiance of wavelength (350+82*10)= 1070 nm**
2.489993	**----------Irradiance of wavelength (350+83*10)= 1080 nm**
2.474348	**----------Irradiance of wavelength (350+84*10)= 1090 nm**
2.460915	**----------Irradiance of wavelength (350+85*10)= 1100 nm**
5	**---------- end flag**

D300.DAT at c:\program files\BWTEK\BWSpec 4\ Files \ Irradiance\Source\ Lamp Data\

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